Eco-profile

of toluene diisocyanate (TDI)

and methylene diphenyl diisocyanate (MDI)

April 2021

CONTENTS

1 SUMMARY

This Eco-profile has been prepared according to **Eco-profiles program and methodology –PlasticsEurope – V3.0 (2019)**.

It provides environmental performance data representative of the average European production of Toluene diisocyanate (TDI) and methylene diphenyl diisocyanate (MDI), from cradle to gate (from crude oil extraction to granulates or resin at plant).

Please keep in mind that comparisons cannot be made on the level of the isocyanate material alone: it is necessary to consider the full life cycle of an application in order to compare the performance of different materials and the effects of relevant life cycle parameters. It is intended to be used by member companies, to support product-orientated environmental management; by users of plastics, as a building block of life cycle assessment (LCA) studies of individual products; and by other interested parties, as a source of life cycle information.

1.1 META DATA

Data Owner	ISOPA
LCA Practitioner	Sphera Solutions GmbH
Programme Owner	PlasticsEurope
Reviewer	DEKRA Assurance Services GmbH, Angela Schindler
Number of plants included in data collection	3 (TDI production) 6 (MDI production)
Representativeness	100 % coverage in terms of production volumes
Reference year	2018
Year of data collection and calculation	2020
Expected temporal validity	2026
Cut-offs	No significant cut-offs
Data Quality	Very good
Allocation method	Combined Elemental + Mass allocation

1.2 DESCRIPTION OF THE PRODUCT AND THE PRODUCTION PROCESS

This EPD is for toluene diisocyanate (TDI) and methylene diphenyl diisocyanate (MDI), diisocyanates used in the production of polyurethanes. The term isocyanate refers to the –N=C=O functional group of one carbon, one nitrogen and one oxygen atoms. Diisocyanates are compounds containing two isocyanate groups.

When a diisocyanate compound is reacted with a compound containing two or more hydroxyl groups (a polyol), long polymer chains are formed, known as polyurethanes.

Toluene diisocyanate (TDI) is mainly used in the industrial manufacture of flexible polyurethane foams while methylene diphenyl diisocyanate (MDI) is used to produce rigid, flexible or elastomeric polyurethane foams.

A combination of the different building blocks can be used for a variety of other polyurethane applications. (see Eco-profile Long and Short Chain Polyether Polyols Polyurethane Products)

The reference flows, to which all data given in this EPD refer, is 1 kg of TDI and 1 kg of MDI.

Production Process

Toluene is the primary raw material for industrial TDI manufacture. To produce TDI, toluene is firstly nitrated with mixed acid to produce a mixture of 2,4- and 2,6-dinitrotoluene isomers. Catalytic reduction of the dinitrotoluene mix produces a corresponding mix of diaminotoluenes (TDA), which are subsequently treat-ed with phosgene to produce TDI.

In the production of MDI, methylenedianiline (MDA) is formed firstly through the reaction of formaldehyde with aniline in the presence of a hydrochloric acid catalyst. Phosgene is reacted with the separated MDA to produce crude MDI, which is then purified.

1.3 DATA SOURCES AND ALLOCATION

The main data source was a data collection from European producers of TDI and MDI. Primary data on gate-to-gate TDI and MDI production is derived from site-specific information for processes under operational control supplied by the participating companies of this study.

Three different TDI producers with three plants in two different European countries participated in the primary data collection.

In the case of MDI five different MDI producers with six plants in five European countries participated in the primary data collection.

In both cases about 100% of the European TDI and MDI production (EU-28) in 2018 are covered, respectively.

The data for the upstream supply chain until the precursors, as well as all relevant background data such as energy and auxiliary material are taken from the GaBi 2020 LCI database [SPHERA 2020]. Most of the background data used is publicly available and public documentation exists.

A partly elemental, partly mass based approach has been chosen for the allocation of the environmental burden of both the production process of TDI and MDI as hydrogen chloride (HCl 100%) results as co-product from both systems. The choice on this allocation procedure took two important aspects into consideration:

- Although the primary purpose of both plants are to produce TDI and MDI, these processes have been specifically designed not only to produce MDI/TDI in the required quality, but also to produce HCl in a quality that can be marketed, i.e. HCl is a desired co-product. Therefore, the quality of the HCl is a critical aspect and influences the process design.
- Despite the fact that both products are sold as valuable substances, prices do not reach the same level for both cases, with higher absolute values for TDI and MDI. But as HCl would have to be neutralized and disposed as a waste if it was not sold as product, the actual value of HCl cannot be expressed by the market value alone. Apart from that market values are volatile and can be very different in different regions.

As a consequence of this a physical allocation approach has been considered to better reflect more the reality - however, a pure mass allocation of all consumed materials would not reflect the elemental reality of both by-products. It also leads to a significantly higher result for HCl compared to its on-purpose production process (using hydrogen and chlorine gas).As in both production processes the main pre-cursors MDA and TDA react with on-site produced phosgene (made from carbon monoxide and chlorine gases) it has been decided to allocate CO (as well as MDA/TDA) to MDI/TDI only and the consumed Chlorine only to HCl.

All other raw materials and energy, (waste) water, waste and emissions are allocated by mass. This approach is called “combined elemental + mass allocation” in the following.

Use Phase and End-of-Life Management

Flexible polyurethane foams produced from TDI or MDI and polyether polyols are typically used in upholstery, mattresses and automotive seats.

Rigid polyurethane foams produced from MDI and polyether polyols have good thermal insulation properties and are used in the manufacture of freezers and refrigerators, and in building and automotive applications.

Post-consumer recycling of polyurethane products becomes a practice in more and more countries for applications where high volumes are available and which could include collection and sorting. A range of mechanical (regrinding, bonding, pressing, and moulding) and chemical (glycolysis, hydrolysis, pyrolysis) recycling technologies are available to produce alternative products and chemical compounds for subsequent domestic, industrial and chemical applications.

For all post-consumer polyurethane waste, for which recycling has not proven to be economically feasible due to contamination and/or complex collection and/or dismantling steps (e.g. automotive shredding), energy recovery is still the option of choice. However, as society moves towards a circular economy in the coming decades the level of energy recovery will decrease and increasingly more sectors will initiate recycling projects for post-consumer PU waste.

1.4 Environmental Performance

The tables below show the environmental performance indicators associated with the production of 1 kg of TDI and MDI, respectively.

1.4.1 Input Parameters

Indicator	Unit	Value		Impact method ref.
		MDI	TDI	
Non-renewable energy resources[1)]				
• Fuel energy	MJ	55.76	56.90	-
• Feedstock energy	MJ	27.60	22.40	Gross calorific value
Renewable energy resources (biomass)[1)]				
• Fuel energy	MJ	1.84	2.21	-
• Feedstock energy	MJ	0.00	0.00	Gross calorific value-
Abiotic Depletion Potential				
• Elements	kg Sb eq.	1.78E-06	9.15E-07	CML 2016
• Fossil fuels	MJ	74.76	71.12	CML 2016
Renewable materials (biomass)	kg	2.52E-12	2.29E-12	
Water	kg			
• Use	kg	906.03	1129.65	-
• Consumption	kg	12.16	9.32	-
[1)] Calculated as upper heating value (UHV)				

1.4.2 Output Parameters

Indicator	Unit	Value		Impact method ref.
		MDI	TDI	
GWP	kg CO_2 eq.	2.76	3.14	CML 2016
ODP	g CFC-11 eq.	7.95E-12	1.10E-11	CML 2016
AP	g SO_2 eq.	3.19	3.33	CML 2016
POCP	g Ethene eq.	0.55	0.89	CML 2016
EP	g PO_4^{3-} eq.	0.59	0.75	CML 2016
Dust/particulate matter[2)]	g PM10	0.10	0.07	-
Total particulate matter[2)]	g	0.14	0.11	-
Waste				
• Non-hazardous	kg	0.03	0.05	-
• Hazardous	kg	6.75E-04	6.15E-04	-
[2)] Including secondary PM10				

1.5 ADDITIONAL ENVIRONMENTAL AND HEALTH INFORMATION

This part has been written under the responsibility of the Data owner only and is not part of the LCA practitioner and reviewer work.

The manufacturers of MDI and TDI are working through ISOPA to promote Product Stewardship and responsible practice in the value chain. These activities include driver training, tank farm assessments and HSE training in the use of MDI and TDI through the “Walk the Talk” programme.

The EU introduces mandatory training of diisocyanates workers from 24 August 2023 in new REACH Restriction the restriction on diisocyanates introduces new minimum training requirements for workers handling diisocyanates and mixtures containing diisocyanates.

ISOPA and their member companies welcome the restriction which is an important step to enhance and harmonise the level of protection of workers using diisocyanates across the EU.

The restriction will apply from 24 August 2023 after a transition period of three years, and ISOPA together with other industry-associations are developing a comprehensive package of training materials for the industrial and professional value chains.

The industry agrees with ECHA’s assessment that the restriction is the most effective and efficient measure to enhance occupational health and safety.

The restriction establishes requirements for the use and placing on the market of diisocyanates as substances on their own, as a constituent in other substances or in mixtures for industrial and professional use(s) in concentrations above 0,1% by weight.

Specifically, the restriction establishes:

- Minimum requirements for training to be provided to industrial and professional users without prejudice to stricter national obligations in the member States.
- Requirements for diisocyanate suppliers to provide training materials in the official language(s) of the member state(s) where they supply the substance(s) or mixture(s);
- Obligation to include information on training requirements on the packaging by suppliers of diisocyanates.
- Mandatory documentation by the employer or self-employed of the successful completion of the training which must be renewed at least every five years.
- Obligation for member states to report on progress and impact of the restriction.

ISOPA and its members are committed to working with stakeholders and authorities to make available the training and courses across the EU in all Member State languages.

1.6 Additional Technical Information

This part has been written under the responsibility of the Data owner only and is not part of the LCA practitioner and reviewer work.

MDI and TDI are raw materials for polyurethane materials. The intrinsic product qualities of polyurethanes are lightweight; strong; durable; resistant to abrasion and corrosion. In addition, polyurethane insulation materials in building applications, refrigerators and freezers enable very large energy savings in heating & cooling to be made.

1.7 Additional Economic Information

This part has been written under the responsibility of the Data owner only and is not part of the LCA practitioner and reviewer work.

MDI and TDI are raw materials for polyurethane materials. Polyurethane materials find wide application as coatings, flexible foams, rigid foams and elastomers. Fields of application include construction, transport, clothing, shoes, bedding, furniture, refrigerators and freezers.

1.7.1 Programme Owner

PlasticsEurope

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B-1040 Brussels, Belgium

E-mail: info@plasticseurope.org

For copies of this EPD, for the underlying LCI data (Eco-profile); and for additional information, please refer to http://www.plasticseurope.org/.

1.7.2 Data Owner

ISOPA Aisbl

Rue Belliard 65

B-1040 Brussels, Belgium

E-mail: main@isopa.org

1.7.3 LCA practitioner

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70771 Leinfelden-Echterdingen, Germany

Tel.: +49 711 3418170

1.7.4 Reviewer

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Handwerkstr. 15

70565 Stuttgart, Germany

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2 ECO-PROFILE REPORT

2.1 FUNCTIONAL UNIT AND DECLARED UNIT

TDI: 1 kg of primary toluene diisocyanate (TDI) »at gate« (production site output) representing a European industry production average.

MDI: 1 kg of primary methylene diphenyl diisocyanate (MDI) »at gate« (production site output) representing a European industry production average.

2.2 PRODUCT DESCRIPTION

Toluene diisocyanate (TDI) and methylene diphenyl diisocyanate (MDI) are organic isocyanates used as key inputs together with polyols to the industrial-scale production of polyurethanes.

Toluene diisocyanate (TDI)

- IUPAC name: 2,4-Diisocyanato-1-methylbenzene
- CAS numbers covered in this study: 26471-62-5, 584-84-9, 110839-12-8, 26603-40-7
- chemical formula: $C_9H_6N_2O_2$
- gross calorific value: 22.4 MJ/kg

Methylene diphenyl diisocyanate (MDI)

- IUPAC name: 1,1'-Methylenebis(4-isocyanatobenzene)
- CAS numbers covered in this study: 101-68-8, 5873-54-1, 25686-28-6, 32055-14-4, 75880-28-3, 88288-99-7, 123714-19-2, 161074-84-6, 2536-05-2,109331-54-6, 58067-54-2
- chemical formula: $C_{15}H_{10}N_2O_2$
- gross calorific value: 27.6 MJ/kg

2.3 MANUFACTURING DESCRIPTION

Toluene diisocyanate (TDI)

TDI is mainly used in the manufacture of flexible polyurethane foams used in upholstery, mattresses and automotive seats. Other uses for TDI include polyurethane elastomers and coatings.

Commercial synthesis of TDI takes place in closed systems and involves the following major stages:

- Nitration of toluene to dinitrotoluene (DNT): The nitration of toluene to DNT is achieved by the reaction of toluene with nitric acid and a catalyst. Toluene is di-nitrated to an approximate 80% : 20% mixture of 2,4-DNT and 2,6-DNT isomers.

- Hydrogenation of DNT to the corresponding diaminotoluenes (TDA): Catalytic reduction of dinitrotoluene under hydrogen pressure is subsequently undertaken to produce diaminotoluene (TDA).

- Phosgenation of TDA: TDA is treated with phosgene under controlled temperature and pressure conditions, resulting in a TDI isomer mixture in solution, together with traces of phosgene and HCl. These traces are subsequently separated and recycled.

- TDI purification: The TDI isomer mixture is then purified by distillation. There is no change to the 80% : 20% isomer composition during this step.

- TDI Differentiation: Both 100 % 2,4-TDI as well as a 65 % : 35 % mixture of 2,4- and 2,6-TDI are produced by separation of the purified 80 % : 20 % TDI.

Methylene diphenyl diisocyanate (MDI)

While MDI exists in three isomers, 4.4-MDI is the most widely used in industrial and is the one represented in this report. The major application of 4.4-MDI is as a primary feedstock for the production of rigid polyurethane foams. Such foams have good thermal insulation properties and are used worldwide in the manufacture of freezers and refrigerators, and in building and automotive applications. Commercial production of MDI involves the following key process stages.

The production of MDI involves the following major stages:

- Production of methylenedianiline (MDA): In the production of MDI, methylenedianiline (MDA) is formed initially through the reaction of formaldehyde with aniline in the presence of a hydrochloric acid catalyst. The percentage distribution of isomers of MDA formed during this step depends on the ratio of aniline to formaldehyde, the acid concentration, and the reaction conditions. After the reaction, the mixture is neutralised by adding caustic soda, and separates into an organic phase and an inorganic (aqueous) phase. The organic phase containing crude MDA is washed. Excess aniline from washing is isolated by distillation for recycling in the first step of the reaction. The inorganic (aqueous) phase is purified from any residual organics and discharged for further treatment or recovery.

- Phosgenation of MDA to crude MDI: During this stage phosgene is reacted with MDA in an inert solvent to produce crude MDI and a hydrogen chloride by-product.

• Solvent Recovery and MDI Purification: Following phosgenation, when evolution of hydrogen chloride is complete and a homogeneous solution is obtained, the solvent is recovered by distillation. Purified MDI is obtained by fractional distillation, crystallization, or sublimation.

2.4 Producer Description

The following companies have participated to the data collection.

Eco-profiles and EPDs represent European industry averages within the scope of ISOPA as the issuing trade federation. Hence, they are not attributed to any single producer, but rather to the European plastics industry as represented by ISOPA's membership and the production sites participating in the Eco-profile data collection. The following companies contributed data to this Eco-profile and EPD:

• BASF Polyurethanes GmbH

Elastogranstraße 60

PO Box 1140

D-49448 Lemförde

Germany

www.polyurethanes.basf.de

• Covestro

Covestro Deutschland AG

51373 Leverkusen

Gemany

https://www.covestro.com/

• BorsodChem

Bolyai tér 1.

H-3700 Kazincbarcika

Hungary

www.borsodchem-pu.com

- Huntsman

Everslaan 45

B-3078 Everberg

Belgium

www.huntsman.com/pu

- Dow Europe GmbH

Bachtobelstrasse 3

CH-8810 Horgen

Switzerland

www.dow.com

2.5 SYSTEM BOUNDARIES

PlasticsEurope Eco-profiles and EPDs refer to the production of polymers as a cradle-to-gate system (see Figure 1 for TDI and Figure 2 for MDI):

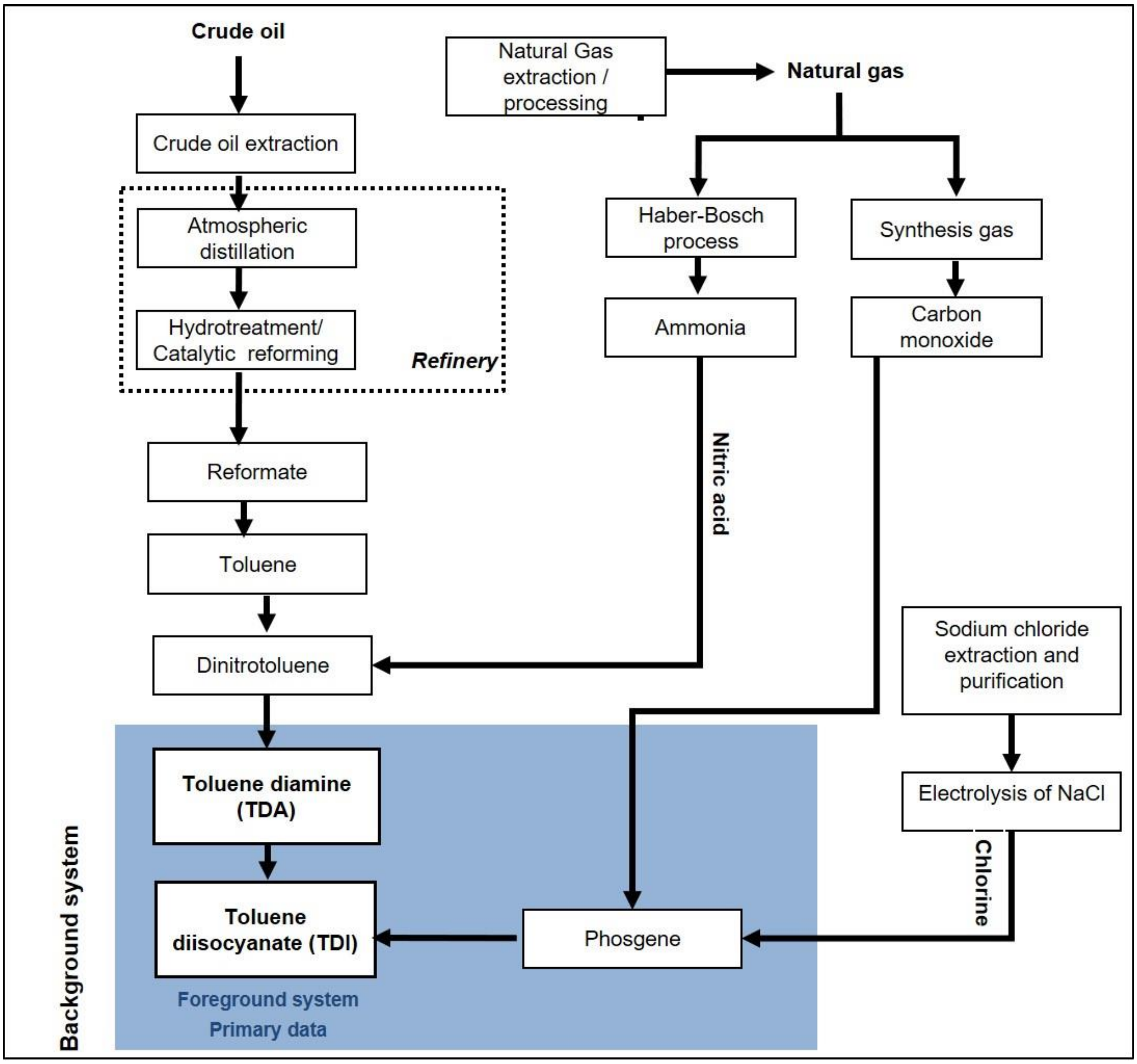

Figure 1: Cradle-to-gate system boundaries (TDI)

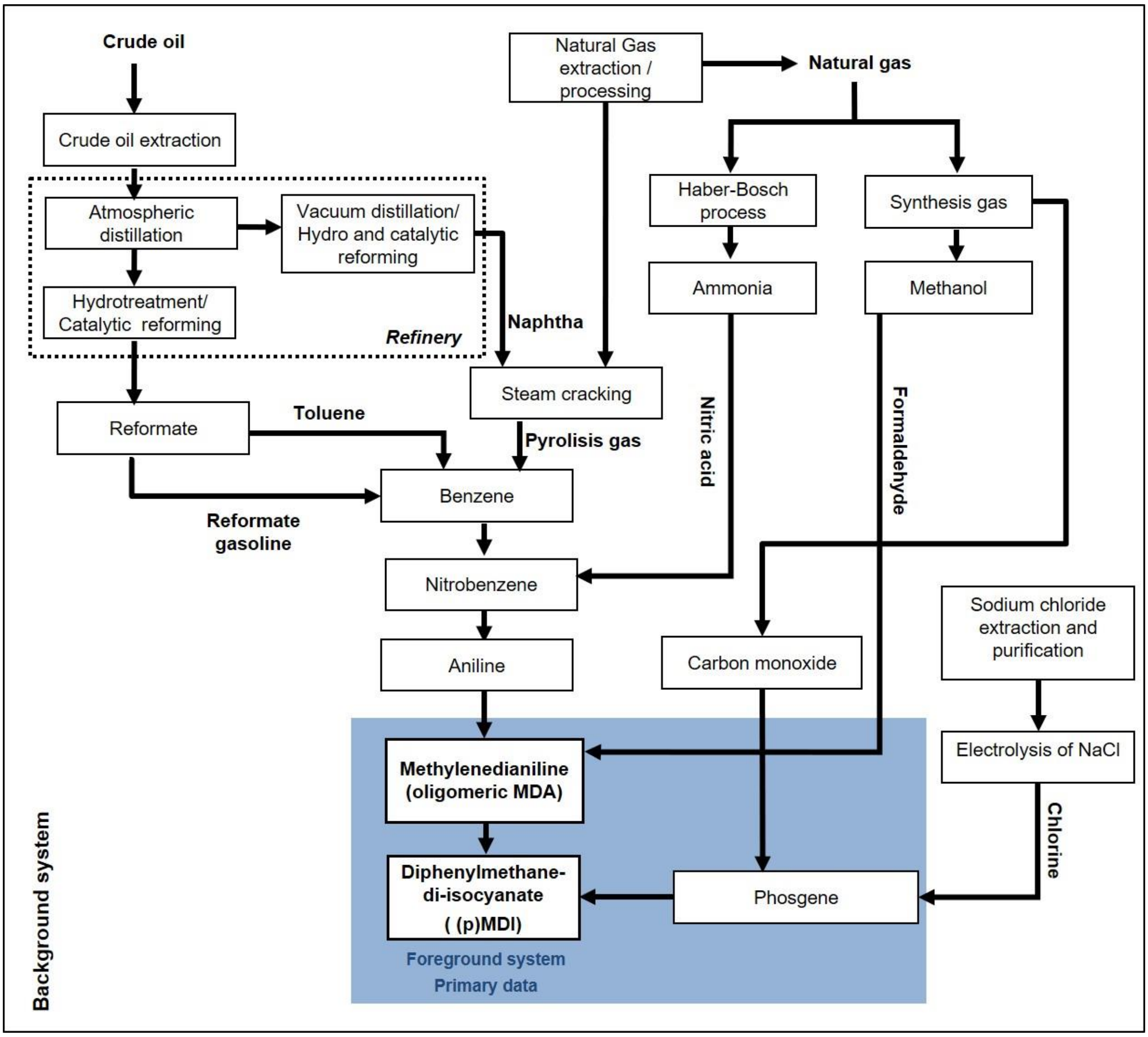

Figure 2: Cradle-to-gate system boundaries (MDI)

2.6 Technological Reference

The production processes were modelled using specific values from primary data collection at site, representing the specific technology for the five companies. The LCI data represent technology in use in the defined production region employed by participating producers. The considered participants cover 100% of the European production in 2018.

Primary data were used for all foreground processes (under operational control) complemented with secondary data from background processes (under indirect management control).

2.7 TEMPORAL REFERENCE

The LCI data for production was collected as 12-month averages representing the year 2018, to compensate for seasonal influence of data.

Background data have reference year from 2019. The dataset is considered to be valid until substantial technological changes in the production chain occur. Having the latest technology development in mind, the companies participating in this Eco-profile define as temporal reference: the overall reference year for this Eco-profile is 2018 with a recommended temporal validity until 2026.

2.8 GEOGRAPHICAL REFERENCE

Primary production data for the TDI production is from three different suppliers in the EU. For MDI, production data is from five suppliers. Fuel and energy inputs in the system reflect average European conditions and whenever applicable, site specific conditions were applied, to reflect representative situations. Therefore, the study results are intended to be applicable within EU boundaries and in order to be applied in other regions adjustments might be required. TDI and MDI imported into Europe was not considered in this Eco-profile.

2.9 CUT-OFF RULES

In the foreground processes all relevant flows were considered, trying to avoid any cut-off of material and energy flows. In single cases additives used in the MDI and/or TDI unit process (<0.1 % m/m of product output) were neglected. In all cases it was assured that no hazardous substances or metals were present in this neglected part.

According to the GaBi 2020 LCI database [SPHERA 2020], used in the background processes, at least 95% of mass and energy of the input and output flows were covered and 98% of their environmental relevance (according to expert judgment) was considered, hence an influence of cut-offs less than 1% on the total is expected. All transports in the pre-chain contribute maximum 0.2% to the overall environmental burden. Including production, the contribution of all transports is expected to be less than 1

2.10 DATA QUALITY REQUIREMENTS

Data Sources

Eco-profiles and EPDs developed by ISOPA use average data representative of the respective foreground production process, both in terms of technology and market share. The primary data are derived from site specific information for processes under operational control supplied by the participating member companies of ISOPA (see Producer Description). The data for the upstream supply chain are taken from the GaBi 2020 LCI database [SPHERA 2020], of the software system GaBi 10.

All relevant background data such as energy and auxiliary material are also taken from the GaBi 2020 LCI database [SPHERA 2020]. Most of the background data used is publicly available and public documentation exists.

Relevance

Regarding the goal and scope of this Eco-profile, the collected primary data of foreground processes are of high relevance, i.e. data was sourced from the most important TDI and MDI producers in Europe in order to generate a European industry average. The environmental contributions of each process to the overall LCI results are included in the Chapter 'Dominance Analysis'.

Representativeness

The considered participants covered 100% of the MDI and TDI European production in 2018, respectively. The selected background data can be regarded as representative for the intended purpose, as it is average data

Consistency

To ensure consistency only primary data of the same level of detail and background data from the GaBi 2020 LCI database [SPHERA 2020] were used. While building up the model, cross-checks concerning the plausibility of mass and energy flows were continuously conducted. The methodological framework is consistent throughout the whole model as the same methodological principles are used both in foreground and background system.

Reliability

Data reliability ranges from measured to estimated data. Data of foreground processes provided directly by producers were predominantly measured. Data of relevant background processes were measured at several sites or determined by literature data or estimated for some flows, which usually have been reviewed and checked for its quality.

Completeness

Primary data used for the gate-to-gate production of MDI and TDI covers all related flows in accordance with the cut off criteria. In this way all relevant flows were quantified, and data is considered complete.

Precision and Accuracy

As the relevant foreground data is primary data or modelled based on primary information sources of the owner of the technology, better precision is not reachable within this goal and scope. All background data is consistently GaBi professional data with related public documentation.

Reproducibility

All data and information used are either documented in this report or they are available from the processes and process plans designed within the GaBi 10 software. The reproducibility is given for internal use since the owners of the technology provided the data and the models are stored and available in a database. Sub-systems are modelled by ´state of art´ technology using data from a publicly available and internationally used database. It is worth noting that for external audiences, it may be the case that full reproducibility in any degree of detail will not be available for confidentiality reasons. However, experienced experts would easily be able to recalculate and reproduce suitable parts of the system as well as key indicators in a certain confidence range.

Data Validation

The data on production collected from the project partners and the data providing companies was validated in an iterative process several times. The collected data was validated using existing data from published sources or expert knowledge.

The background information from the GaBi 2020 LCI database [SPHERA 2020] is updated regularly and validated and benchmarked daily by its various users worldwide.

Life Cycle Model

The study has been performed with the LCA software GaBi 10. The associated database integrates ISO 14040/44 requirements. Due to confidentiality reasons details on software modelling and methods used cannot be shown here. However, in principle the model can be reviewed in detail if the data owners agree. The calculation follows the vertical calculation methodology, i.e. that the averaging is done after modelling the specific processes.

2.11 CALCULATION RULES

Vertical Averaging

When modelling and calculating average Eco-profiles from the collected individual LCI datasets, vertical averages were calculated (Figure 3).

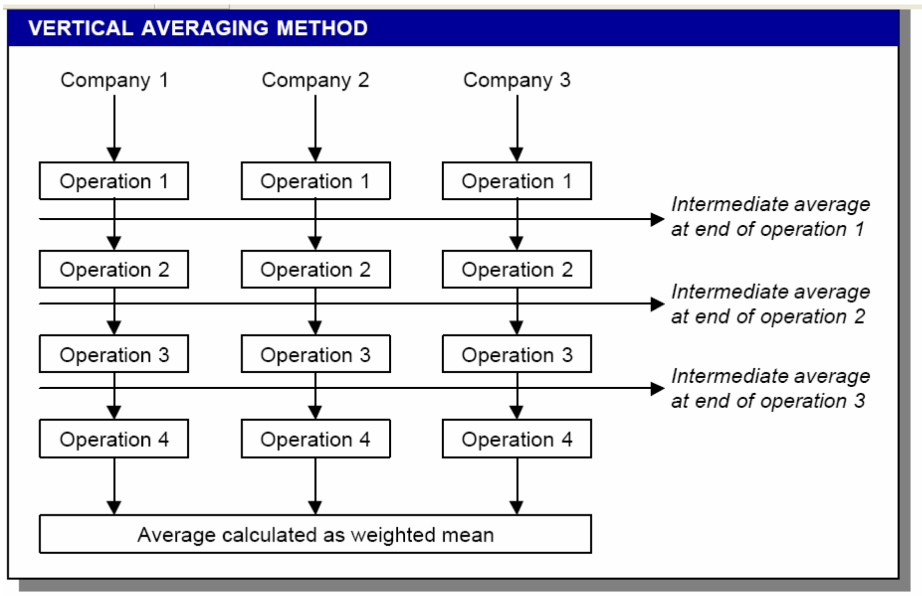

Figure 3: Vertical Averaging (source: Eco-profile of high-volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001)

Allocation Rules

Production processes in chemical and plastics industry are usually multi-functional systems, i.e. they have not one, but several valuable product and co-product outputs. Wherever possible, allocation should be avoided by expanding the system to include the additional functions related to the co-products. Often, however, avoiding allocation is not feasible in technical reality, as alternative stand-alone processes are not existing, or alternative technologies show completely different technical performance and product quality output. In such cases, the aim of allocation is to find a suitable partitioning parameter so that the inputs and outputs of the system can be assigned to the specific product sub-system under consideration.

For TDI and MDI processes, in which hydrogen chloride (HCl) results as co-product for both processes, allocation turns to be a very sensitive issue.

As shown in Table 1, depending on the allocation procedure adopted and taking the combined elemental + mass allocation approach (as described in chapter 1.3) as a base case, TDI results for GWP might increase by 46% with price allocation and decrease by 21.5 % when applying 100% mass allocation. Considering the total primary energy demand price allocation would lead to an increase of 37%, whereas mass allocation would show a decrease of 25,2%.

Similar observation can be made for MDI with an potential increase of 22% (price allocation) respectively decrease of 15,8% (mass allocation) for GWP while regarding the total primary energy demand a 15% increase (price) and 20,5% decrease (mass) could be observed (Table 2).

Table 1: Allocation procedures (system boundary level) per 1kg TDI

Environmental Impact Category	Elemental + Mass Allocation	Mass allocation	Price allocation
Global Warming Potential (GWP) [kg CO_2 eq]	3.14	2.49	4.59
Gross primary energy from resources [MJ]	74.9	56	103

Table 2: Allocation procedures (system boundary level) per 1kg MDI

Environmental Impact Category	Elemental + Mass Allocation	Mass allocation	Price allocation
Global Warming Potential (GWP) [kg CO_2 eq]	2.76	2.32	3.37
Gross primary energy from resources [MJ]	78.3	62.5	90.8

In all cases the allocation procedure refers as by-product HCl as 100% and not its solution.

The following table shows for informational purposes the respective indicator results for the HCl gained as by-product (applying Elemental+Mass allocation) next to the results of its on-purpose production (source: GaBi database, country: Germany)

Table 3: LCA results of HCl (100%) as by-product of TDI, MDI and from on-purpose production

Environmental Impact Category	By-Product of TDI	By-Product of MDI	On-Purpose Production
Global Warming Potential (GWP) [kg CO_2 eq]	1.77	1.44	1.19
Gross primary energy from resources [MJ]	36.8	32.1	27.3

In the refinery operations, co-production was addressed by applying allocation based on mass and net calorific value [SPHERA 2020]. The chosen allocation in refinery is based on several sensitivity analyses, which was accompanied by petrochemical experts. The relevance and influence of possible other allocation keys in this context is small. In steam cracking, allocation according to net calorific value is applied. Relevance of other allocation rules (mass) is below 2 %.

2.12 LIFE CYCLE INVENTORY (LCI) RESULTS

Delivery and Formats of LCI Dataset

This eco-profile comprises

- a dataset in ILCD format (http://lct.jrc.ec.europa.eu) according to the last version at the date of publication of the eco-profile and including the reviewer (internal and external) input.
- This report in pdf format.

Energy Demand

The **primary energy demand** (system input) of 81.51 MJ/kg TDI and 85.20 MJ/kg MDI indicates the cumulative energy requirements at the resource level, accrued along the entire process chain (system boundaries), quantified as gross calorific value (upper heating value, UHV).

The **energy content in the isocyanate** indicates a measure of the share of primary energy incorporated in the product, and hence a recovery potential (system output), quantified as the gross calorific value (UHV), is 22.4 MJ/kg TDI and 27.6 MJ/kg MDI.

The difference (∆) between primary energy input and energy content in the isocyanate output is a measure of **process energy** which may be either dissipated as waste heat or recovered for use within the system boundaries. Useful energy flows leaving the system boundaries were treated with cut -off approach (no credits associated to main product system).

Table 3 Primary energy demand (system boundary level) per 1kg TDI

Primary Energy Demand	Value [MJ]
Energy content in polymer (energy recovery potential, quantified as gross calorific value of monomer)	22.40
Process energy (quantified as difference between primary energy demand and energy content of monomer)	59.11
Total primary energy demand	**81.51**

Table 4 Primary energy demand (system boundary level) per 1kg MDI

Primary Energy Demand	Value [MJ]
Energy content in polymer (energy recovery potential, quantified as gross calorific value of monomer)	27.60
Process energy (quantified as difference between primary energy demand and energy content of monomer)	57.60
Total primary energy demand	**85.20**

Water cradle to gate Use and Consumption

The cradle-to-gate water use is 1129.65 kg for TDI and 906.03 kg for MDI, respectively. The corresponding water consumption in the same system boundary is 12.16 kg (TDI) and 9.32 kg (MDI)

Water foreground (gate to gate) Use and Consumption

The following tables show the weighted average values for water use of the TDI and MDI production process (gate-to-gate level). For each of the typical water applications the water sources are shown.

Table 5 Water use and source per 1kg of TDI

Source	Process water [kg]	Cooling water [kg]	Steam Water [kg]	Water in Raw Materials [kg]	Total [kg]
From Tap	0.00	2.35	0.00	0.00	**2.35**
Deionized / Softened	0.20	0.00	2.36	0.09	**2.64**
Untreated (from river/lake)	1.40	21.40	0.00	0.00	**22.80**
Untreated (from sea)	0.00	0.00	0.00	0.00	**0.00**
Relooped	0.00	69.68	0.11	0.00	**69.80**
Totals	**1.60**	**93.44**	**2.47**	**0.09**	**97.59**

Table 6 Water use and source per 1kg of MDI

Source	Process water [kg]	Cooling water [kg]	Steam Water [kg]	Water in Raw Materials [kg]	Total [kg]
From Tap	0.00	0.00	0.00	0.00	**0.00**
Deionized / Softened	0.53	0.18	1.04	0.19	**1.95**
Untreated (from river/lake)	0.34	2.80	0.00	0.00	**3.14**
Untreated (from sea)	0.00	0.00	0.00	0.00	**0.00**
Relooped	0.03	65.21	0.01	0.00	**65.25**
Totals	**0.90**	**68.19**	**1.05**	**0.19**	**70.34**

The following tables show the further handling/processing of the water output of the production process of TDI and MDI.

Table 7 Treatment of Water Output per 1kg of TDI

Treatment	Water Output [kg]
To WWTP	1.62
Untreated (to river/lake)	21.40
Untreated (to sea)	0.00
Relooped	71.59
Water leaving with products	0.00
Water Vapour	2.98
Formed in reaction (to WWTP)	0.37
Totals	**97.97**

Table 8 Treatment of Water Output per 1kg of MDI

Treatment	Water Output [kg]
To WWTP	1.09
Untreated (to river/lake)	2.39
Untreated (to sea)	0.07
Relooped	66.01
Water leaving with products	0.00
Water Vapour	0.78
Formed in reaction (to WWTP)	0.07
Totals	**70.41**

Based on the water use and output figures above the **water consumption** can be calculated as:

Consumption = (water vapour + water lost to the sea) – (water generated by using water containing raw materials + water generated by the reaction + seawater used)

- TDI = 2.52 kg
- MDI = 0.58 kg

Dominance Analysis

Table 7 and Table 8 show the main contributions to the results presented above. An average based on the weighted mean from the different technologies of the participating producers is used.

Looking at the TDI results is can be observed that in all analysed environmental impact categories, the intermediates (Nitric Acid + Toluene + other chemicals) contribute to at least 75 % or more of the total impact, except for ODP which is dominated by the electricity consumption. The remaining impact categories are dominated by Nitric Acid + Toluene, except for ADP elements which is influenced significantly by other raw materials.

With regards to the MDI results it can be stated that in all analysed environmental impact categories, intermediates (Aniline + other chemicals) contribute to at least 70 % or more of the total impact. While the burden is almost shared equally regarding ODP, the indicator ADP elements is dominated by raw materials other than Aniline. The latter one is, in contrary, responsible for at least 50% of the total burden in all remaining indicators covered in this study.

The use of high-quality data especially for this case is therefore decisive to the environmental profile of MDI.

Table 9 Dominance analysis of impacts per 1kg TDI

	Total Primary Energy	**ADP elements**	**ADP fossil**	**GWP**	**AP**	**EP**	**POCP**	**ODP**
Production Process	0%	0%	0%	0%	0%	0%	0%	0%
Nitric Acid + Toluene	59%	24%	61%	50%	57%	75%	83%	38%
Other Chemicals	25%	63%	25%	28%	19%	11%	10%	17%
Thermal Energy	10%	5%	11%	15%	7%	6%	4%	0%
Electricity	5%	6%	3%	6%	13%	6%	3%	45%
Utilities	0%	0%	0%	0%	0%	0%	0%	1%
Process Waste Treatment	0%	1%	0%	1%	4%	2%	0%	-1%
Transports	0%	0%	0%	0%	0%	0%	0%	0%
Total	100%	100%	100%	100%	100%	100%	100%	100%

Table 10 Dominance analysis of impacts per 1kg MDI

	Total Primary Energy	**ADP elements**	**ADP fossil**	**GWP**	**AP**	**EP**	**POCP**	**ODP**
Production Process	0%	0%	0%	0%	0%	0%	0%	0%
Aniline	76%	19%	78%	74%	73%	76%	82%	38%
Other Chemicals	16%	78%	15%	13%	16%	14%	12%	33%
Thermal Energy	5%	1%	5%	9%	4%	4%	4%	0%
Electricity	2%	1%	1%	3%	5%	3%	2%	28%
Utilities	0%	1%	0%	0%	0%	0%	0%	1%
Process Waste Treatment	0%	0%	0%	0%	0%	1%	0%	0%
Transports	0%	0%	0%	0%	1%	2%	-1%	0%
Total	100%	100%	100%	100%	100%	100%	100%	100%

Comparison of the present Eco-profile with its previous version

Table 11 Comparison of the present Eco-profile with its previous version for TDI

Environmental Impact Categories	Eco-profile TDI Previous (2012)	Eco-profile TDI New (2021)	Difference (%)
Gross primary energy from resources [MJ]	58.57	81.51	Results not directly comparable due to a different allocation approach (see above)
Abiotic Depletion Potential (ADP), elements [kg Sb eq.]	6.67E-06	9.15E-07	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	48.90	71.12	
Global Warming Potential (GWP) [kg CO_2 eq.]	2.71	3.14	
Acidification Potential (AP) [g SO_2 eq.]	3.87	3.33	
Eutrophication Potential (EP) [g PO_4^{3-} eq.]	0.87	0.75	
Ozone Depletion Potential (ODP) [g CFC-11 eq.]	6.65E-05	1.10E-11[1]	
Photochemical Ozone Creation Potential [g Ethene eq.]	0.64	0.89	

Table 12 Comparison of the present Eco-profile with its previous version for MDI

Environmental Impact Categories	Eco-profile MDI Previous (2012)	Eco-profile MDI New (2021)	Difference (%)
Gross primary energy from resources [MJ]	61.59	85.2	Results not directly comparable due to a different allocation approach (see above)
Abiotic Depletion Potential (ADP), elements [kg Sb eq.]	6.04E-06	1.78E-06	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	53.42	74.76	
Global Warming Potential (GWP) [kg CO_2 eq.]	2.39	2.76	
Acidification Potential (AP) [g SO_2 eq.]	4.30	3.19	
Eutrophication Potential (EP) [g PO_4^{3-} eq.]	0.68	0.59	
Ozone Depletion Potential (ODP) [g CFC-11 eq.]	7.69E-03	7.95E-12[1]	
Photochemical Ozone Creation Potential [g Ethene eq.]	0.68	0.55	

As for both, TDI and MDI, LCA results have been calculated by applying the mass allocation approach as scenario analysis (for GWP and primary energy demand, see above); the respective outcome can be contrasted: it can be stated, that at least regarding those indicators the weighted average production systems have slightly improved (regarding GWP: 8% for TDI, 3% for TDI). However it should be considered as well, that also background

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[1] Since the use of certain halogenated substances has been banned following the implementation of the Montreal Protocol, the following emissions are not present anymore in the updated Sphera datasets: Halon (1301), R 11 (trichlorofluoromethane), R 114 (dichlorotetrafluoroethane) and R 12 (dichlorodifluoromethane) and R22 (chlorodifluoromethane). Particularly R22, which has been removed, has the profound effect of reducing the remaining, already greatly reduced ODP impacts by several orders of magnitude for most datasets. This consequently further reduces the impact results for ODP for many datasets in the database.

datasets become “greener” over time by reflecting on more efficient upstream process technologies and green electricity/energy mixes.

3 REVIEW

3.1 EXTERNAL INDEPENDENT REVIEW SUMMARY

The present Eco-Profile is an update of an Eco-Profile published in 2012 for MDI and TDI.

During the Eco-profile generation by Sphera the question on allocation criteria possibly to be applied for the by-product HCl of the MDI/TDI-production were discussed.
The actual review is based on the final Eco-profile document accompanied by a webmeeting for clarifying open questions and comments of the reviewer, including spot checks of the software model applied and explanations on the primary data collection.

The Eco-profile document was sent and reviewed in March/April 2021.
The compliance of the documents was reviewed according to the current requirements of the Eco-profiles program and methodology, version 3.0 (Oct 2019) of PlasticsEurope and the accompanying template for Eco-profile reports.

The representativeness of the resulting inventory data is estimated according to the expert judgement of ISOPA in respect to the production volumes in Europe. As all main producers have taken part in this study, the technology displays the state-of-the art status.

For the update of the Eco-profile new and complete foreground data were delivered by the participants of the study complemented with upstream process inventories from the current available GaBi database.

The mass allocation approach, applied in the preceding Eco-profile for the by-product HCl by producing the products MDI and TDI were controversially discussed. The current approach of the combined elemental and mass allocation still displays physical reality and reflects more specifically the intention of considered process and products.

The collected data are thoroughly processed; the transfer into a systematically built software model shows a sound quality. The methodological approaches follow the PCR requirements. The recommendations of the reviewer have been followed to clarify certain aspects.

The structure and description of the Eco-profile is clear and transparent, thus displaying a reliable source of information.

So far the PCR does not require specific indicators for the impact assessment. While preparing the life cycle inventory / software model necessary requirements for the assessment of further impact categories, e.g. required by the Product Environmental Footprint were partly integrated, i.e. regionalisation of water flows. Applying the LCI for the assessment of further indicators, not assessed within this Eco-profile, the documentation need to be checked, if respective data are included in the inventory.

3.2 Reviewer Contact Details

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