Eco-profiles and Environmental Product Declarations of the European Plastics Manufacturers

Toluene Diisocyanate (TDI) & Methylenediphenyl Diisocyanate (MDI)

ISOPA

April 2012

PlasticsEurope
Association of Plastics Manufacturers

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Environmental Product Declaration

Introduction

This Environmental Product Declaration (EPD) is based upon life cycle inventory (LCI) data from PlasticsEurope's Eco-profile programme. It has been prepared according to **PlasticsEurope's Eco-profiles and Environmental Declarations – LCI Methodology and PCR for Uncompounded Polymer Resins and Reactive Polymer Precursors** (PCR version 2.0, April 2011). EPDs provide environmental performance data, but no information on the economic and social aspects which would be necessary for a complete sustainability assessment. Further, they do not imply a value judgement between environmental criteria.

This EPD describes the production of the Toluene diisocyanate (TDI) and Methylenediphenyl diisocyanate (MDI) isocyanates from cradle to gate (from crude oil extraction to granules or resin at plant). **Please keep in mind that comparisons cannot be made on the level of the isocyanate 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. This EPD 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.

Meta Data

Data owner	ISOPA
LCA practitioner	PE INTERNATIONAL AG
Programme owner	ISOPA
Programme manager, Reviewer, Database manager	DEKRA Industrial GmbH
Number of plants included in data collection	4 (TDI production) 6 (MDI production)
Representativeness	90 % coverage in terms of production volumes
Reference year	2010
Year of data collection and calculation	2011
Expected temporal validity	2022
Cut-offs	No significant cut-offs
Data quality	Very good
Allocation method	Mass allocation

Description of the Product and the Production Process

This EPD is for Toluene diisocyanate (TDI) and Methylenediphenyl 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 atom. 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 methylenediphenyl 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 treated 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.

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.

Four different TDI producers with plants in three 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 90% of the European TDI and MDI production (EU-27) in 2010 are covered, respectively.

The data for the upstream supply chain until the precursors are taken from the database of the software system GaBi 5 [GaBi 5 2011]. All relevant background data such as energy and auxiliary material are also taken from the GaBi 5 database. Most of the background data used is publicly available and public documentation exists [GaBi 5 2011].

Mass allocation was applied both for the production process of TDI and MDI as hydrogen chloride (HCl 100%) results as co-product from both production processes. The choice on this allocation procedure took two important aspects into consideration:

- Although the primarily 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 on the process design.
- Despite of 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, and therefore the physical procedure (mass allocation) would most reflect the reality.

The final allocation option, the stoichiometric allocation, would not make sense, as it clearly does not reflect the industrial reality and plant purpose, since four moles of HCl are generated per mole MDI or TDI.

In case of minor intermediates to be further used, sold or fuel gas to be applied in combustion processes in specific production processes, allocation was done according to mass, current market prices or energy. A quantified sensitivity analysis was performed whenever different allocation possibilities were applicable.

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 is common for applications where high volumes are available and no, or limited, sorting is necessary. 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 complex collection and/or dismantling steps (e.g. automotive shredding), energy recovery is the option of choice.

Environmental Performance

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

Please note that considering the uncertainty of the exact division of the process energy as originating from either fuels or feedstocks, as well as the use of average data (secondary data) in the modelling with different country-specific grades of crude oil and natural gas, the feedstock and fuel energy are presented as a range.

Input Parameters

Indicator	Unit	Value	
		MDI	TDI
Non-renewable energy resources[1]			
• Fuel energy	MJ	47.20 – 51.20	41.67 – 45.67
• Feedstock energy	MJ	10.4 – 14.4	12.9 – 16.9
Renewable energy resources (biomass)[1]			
• Fuel energy	MJ	1.32	1.32
• Feedstock energy	MJ	-	-
Abiotic Depletion Potential			
• Elements	kg Sb eq	6.04E-06	6.67E-06
• Fossil fuels	MJ	53.42	48.90
Renewable materials (biomass)	kg	–	–
Water use	kg	22	18.2
• for process	kg	3.0	3.1
• for cooling	kg	19.0	15.1
[1] Calculated as upper heating value (UHV)			

Output Parameters

Indicator	Unit	Value	
		MDI	TDI
GWP	kg CO_2 eq	2.39	2.71
ODP	g CFC-11 eq	7,69E-03	6.65E-05
AP	g SO_2 eq	4.30	3.87
POCP	g Ethene eq	0.68	0.64
EP	g PO_4 eq	0.68	0.87
Dust/particulate matter[2]	g PM10	0.055	0.077
Total particulate matter[2]	g	0.21	0.23
Waste			
• Non-hazardous	kg	6.00E-03	8.04E-05
• Hazardous	kg	8.97E-04	3.17E-02
[2] Including secondary PM10			

Additional Environmental and Health Information

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.

Additional Technical Information

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 and cooling to be made.

Additional Economic Information

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.

Information

Data Owner

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B-1160 Brussels, Belgium
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E-mail: main@isopa.org.

Programme Manager & Reviewer

DEKRA Industrial GmbH

This Environmental Product Declaration has been reviewed by DEKRA Industrial GmbH. It was approved according to the Product Category Rules PCR version 2.0 (2011-04) and ISO 14025:2006.

Registration number: PlasticsEurope 2012-0001, valid until 30 April 2015 (date of next revalidation review).

Programme Owner

PlasticsEurope
Avenue E van Nieuwenhuyse 4, Box 3
B-1160 Brussels, Belgium
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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/.

References

- Product photographs on cover with kind permission by BASF AG.
- PlasticsEurope: Eco-profiles and environmental declarations – LCI methodology and PCR for uncompounded polymer resins and reactive polymer precursor (version 2.0, April 2011).

Plastics
The Material for the 21st Century

Goal & Scope

Intended Use and Target Audience

➢ *Eco-profiles (LCIs) and EPDs from this programme are intended to be used as »cradle-to-gate« building blocks of life cycle assessment (LCA) studies of defined applications or products. LCA studies considering the full life cycle (»cradle-to-grave«) of an application or product allow for comparative assertions to be derived. It is essential to note that comparisons cannot be made at the level of the polymer or its precursors. In order to compare the performance of different materials, the whole life cycle and the effects of relevant life cycle parameters must be considered.*

PlasticsEurope Eco-profiles and EPDs represent polymer production systems with a defined output. They can be used as modular building blocks in LCA studies. However, these integrated industrial systems cannot be disaggregated further into single unit processes, such as polymerisation, because this would neglect the interdependence of the elements, e.g. the internal recycling of feedstocks and precursors between different parts of the integrated production sites.

PlasticsEurope Eco-profiles and EPDs are prepared in accordance with the stringent ISO 14040–44 requirements. Since the system boundary is »cradle-to-gate«, however, their respective reference flows are disparate, namely referring to a broad variety of polymers and precursors. This implies that, in accordance with ISO 14040–44, a direct comparison of Eco-profiles is impossible. While ISO 14025, Clause 5.2.2 does allow EPDs to be used in comparison, PlasticsEurope EPDs are derived from Eco-profiles, i.e. with the same »cradle-to-gate« system boundaries.

As a consequence, a direct comparison of Eco-profiles or EPDs makes no sense because 1 kg of different polymers are not functionally equivalent.

Once a full life cycle model for a defined polymer application among several functionally equivalent systems is established, and only then, can comparative assertions be derived. The same goes for EPDs, for instance, of building product where PlasticsEurope EPDs can serve as building blocks.

Eco-profiles and EPDs are intended for use by the following target audiences:

- member companies, to support product-orientated environmental management and continuous improvement of production processes (benchmarking);
- downstream users of plastics, as a building block of life cycle assessment (LCA) studies of plastics applications and products; and
- other interested parties, as a source of life cycle information.

Product Category and Declared Unit

Product Category

The core product category is defined as **uncompounded polymer resins, or reactive polymer precursors**. This product category is defined »at gate« of the polymer or precursor production and is thus fully within the scope of PlasticsEurope as a federation. In some cases, it may be necessary to include one or several additives in the Eco-profile to represent the polymer or precursor »at gate«. For instance, some polymers may require a heat stabiliser, or a reactive precursor may require a flame retardant. This special case is distinguished from a subsequent compounding step conducted by a third-party downstream user (outside PlasticsEurope's core scope).

Functional Unit and Declared Unit

The default Functional Unit and Declared Unit of PlasticsEurope Eco-profiles and EPDs are (unless otherwise specified[1]):

1 kg of primary Toluene diisocyanate (TDI) – or – Methylenediphenyl diisocyanate (MDI) »at gate« (production site output) representing a European industry production average.

Product and Producer Description

Product Description

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

Toluene diisocyanate (TDI)

- 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 of 22.4 MJ/kg.

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.

[1] Exceptions can occur when reporting Eco-profiles of, for instance, process energy, such as on-site steam, or conversion processes, such as extrusion.

Methylenediphenyl diisocyanate (MDI)

- 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, 9016-87-9.
- chemical formula $C_{15}H_{10}N_2O_2$
- gross calorific value of 27.6 MJ/kg.

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.

Producer Description

PlasticsEurope Eco-profiles and EPDs represent European industry averages within the scope of PlasticsEurope as the issuing trade federation. Hence they are not attributed to any single producer, but rather to the European plastics industry as represented by PlasticsEurope'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 Europe
  PO Box 1140
  D-49440 Lemförde
  Germany
  www.polyurethanes.basf.de
- Bayer MaterialScience AG
  D-51368 Leverkusen
  Germany
  www.bayermaterialscience.com
- BorsodChem
  Bolyai tér 1.
  H-3700 Kazincbarcika
  Hungary
  www.borsodchem-pu.com
- Huntsman
  Everslaan 45
  B-3078 Everberg
  Belgium
  www.huntsman.com/pu

- Perstorp
  40 rue de la Haie-Coq
  F-93 306 Aubervilliers Cedex
  France
  www.perstorp.com
- The Dow Chemical Company
  Bachtobelstrasse 3
  CH-8810 Horgen
  Switzerland
  www.dow.com

Life Cycle Inventory

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).

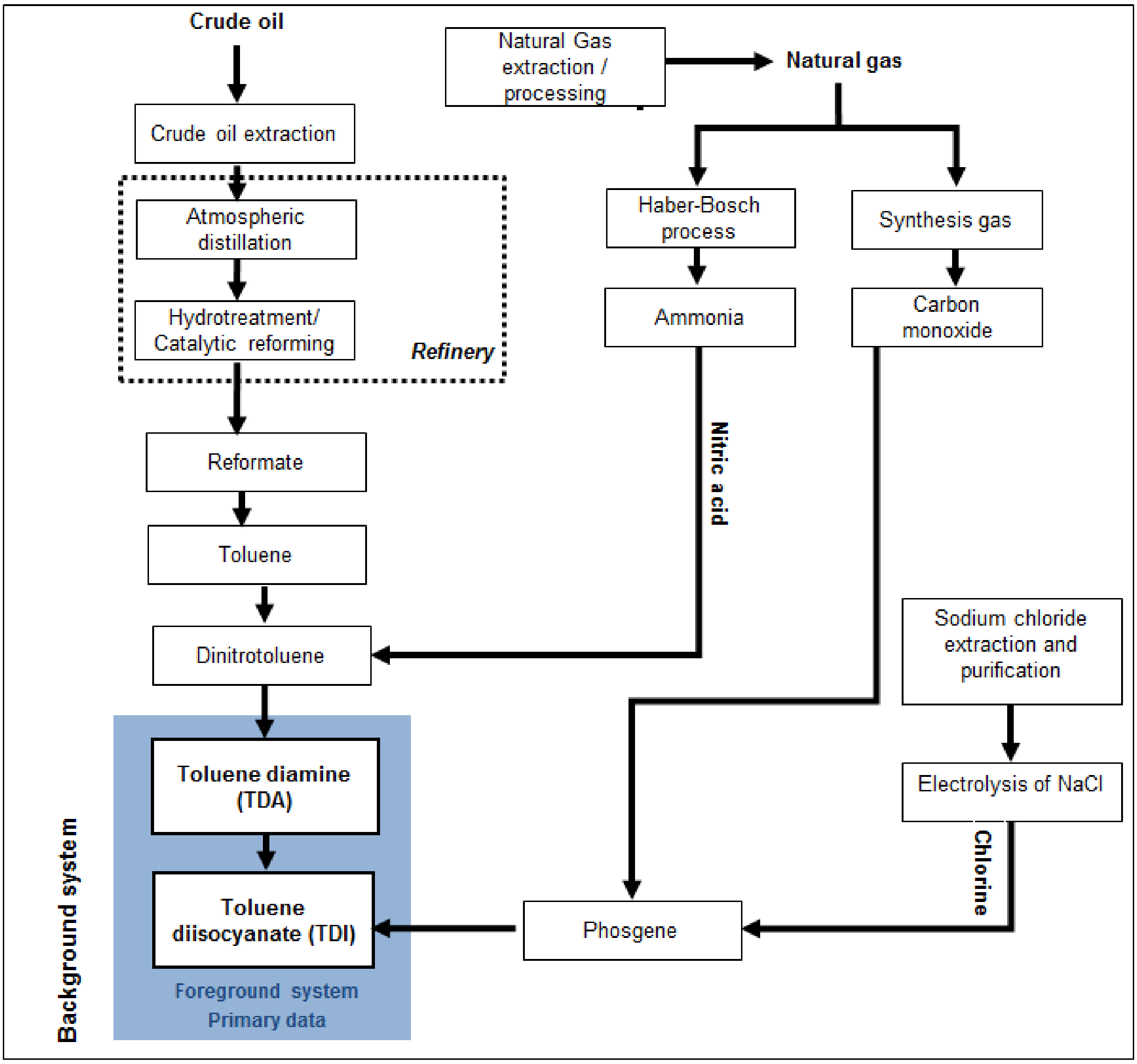


Figure 1: Cradle-to-gate system boundaries (TDI)

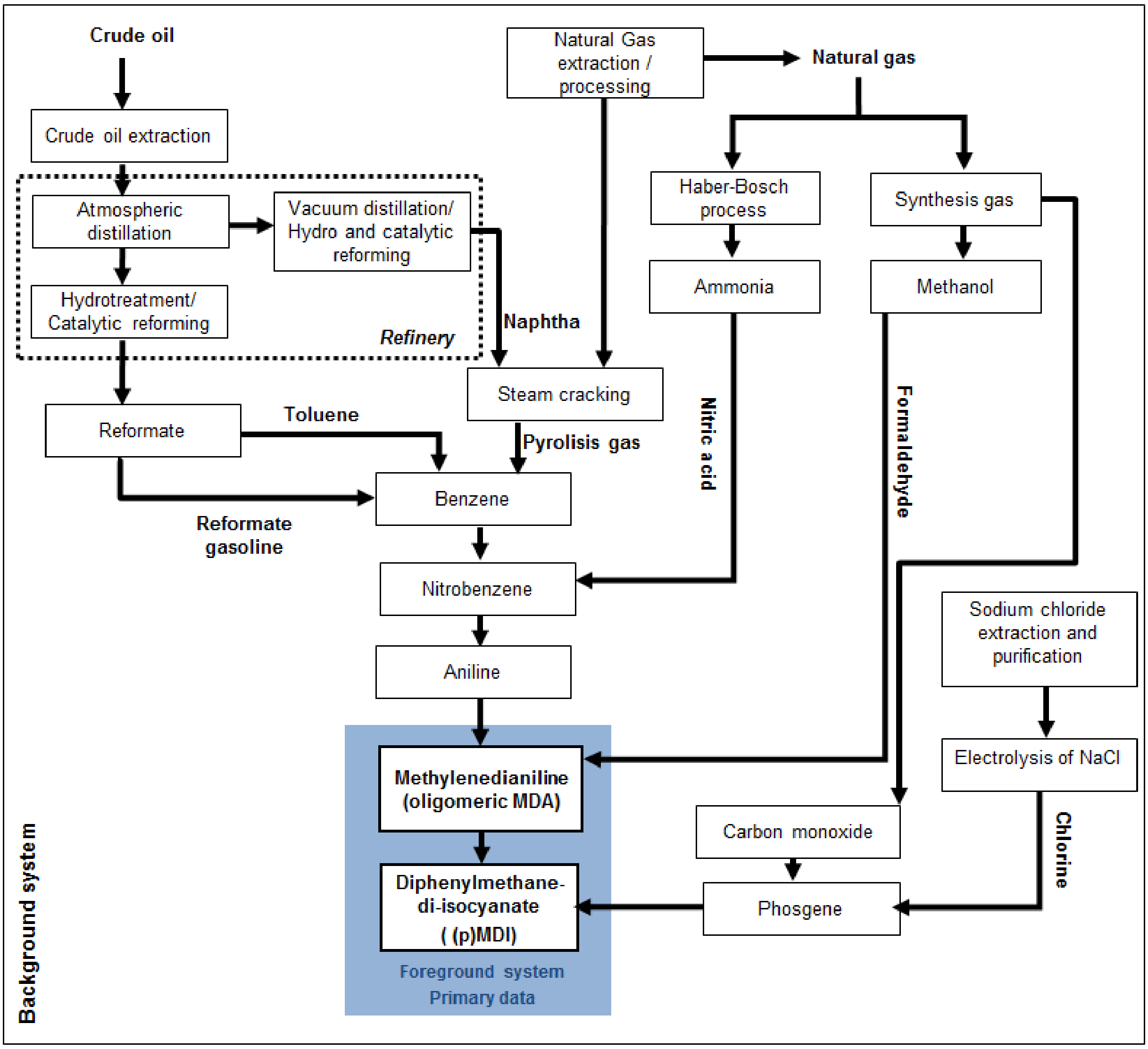


Figure 2: *Cradle-to-gate system boundaries (MDI)*

Technological Reference

The production processes were modelled using specific values from primary data collection at site, representing the specific technology for the six companies. The LCI data represent technology in use in the defined production region employed by participating producers. The considered participants cover 90% of the European production in 2010.

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

Temporal Reference

The LCI data for production was collected as 12 month averages representing the year 2010, to compensate seasonal influence of data.

Background data have reference years from 2010. 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 defines as temporal reference: the overall reference year for this Eco-profile is 2010 with a maximal temporal validity until 2022.

Geographical Reference

Primary production data for the TDI production is from four 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 the Eco-profiles.

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 Databases 2011 [GaBi 5 2011], 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 in 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 %, thus transports are excluded from this investigation.

Data Quality Requirements

Data Sources

Eco-profile 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 life cycle database of the software system GaBi 5 [GaBi 5 2011]. For the most relevant intermediates to the TDI and MDI processes, dinitrotoluene and aniline, respectively, a confirmation of the quality of the data and its industrial representativeness was provided by the participating member companies.

All relevant background data such as energy and auxiliary material are also taken from the GaBi5 database. Most of the background data used is publicly available and public documentation exists. The dominance analysis (Table 37 and Table 38) showed that the contribution of these background datasets without the main intermediates, as mentioned above, on impact indicators is about 30%-40% for MDI and about 40% - 60% for TDI, in both cases with the exception of ADP elements..

Relevance

With regard to 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 ‘ Life Cycle Impact Assessment’.

Representativeness

The considered participants covered 90% of the MDI and TDI European production in 2010, respectively. The selected background data can be regarded as representative for the intended purpose, as it is average data and not in the focus of the analysis.

Consistency

To ensure consistency only primary data of the same level of detail and background data from the GaBi 5 databases [GaBi 5 2011] 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 GaBi5 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 databases 2011 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 5 [GaBi 2011]. The associated database integrate 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.

Calculation Rules

Vertical Averaging

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

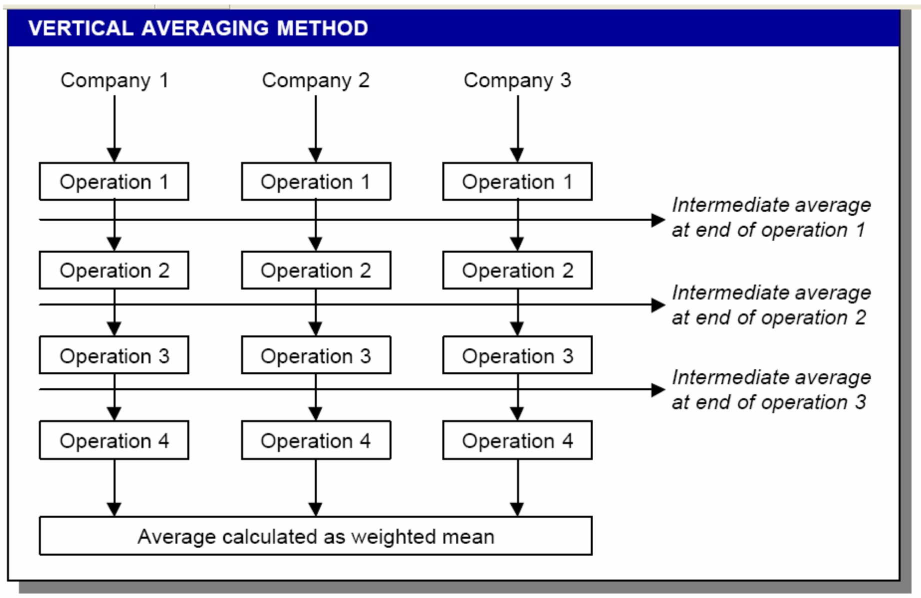


Figure 3: *Vertical Averaging (source: Eco-profile of high volume commodity phthalate esters, ECPI* European *Council for Plasticisers and Intermediates, 2001)*

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 in reality 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 and Table 2, depending on the allocation procedure adopted, taking the mass allocation as a base case, TDI results might increase by 92% (price allocation) and MDI by 55% (price allocation) for both GWP and primary energy.

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

Environmental Impact Category	Mass allocation	Price allocation
Global Warming Potential (GWP) [kg CO_2 eq]	2.71	5.21
Gross primary energy from resources [MJ]	58.57	112.37

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

Environmental Impact Category	Mass allocation	Price allocation
Global Warming Potential (GWP) [kg CO_2 eq]	2.39	3.69
Gross primary energy from resources [MJ]	61.59	95.66

The decision on the most appropriate allocation procedure takes 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 on 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 if not be sold as product, the actual value of HCl cannot be expressed by the market value alone and therefore the physical partitioning (mass allocation) is held to reflect the industrial reality in the best way.

In each case, the allocation procedure refers to HCl (100%) as by-product, not to an aqueous solution.

Stoichiometric allocation was omitted from this sensitive analysis: it does not reflect industrial reality and plant purpose, in that four moles of HCl are generated per mole of MDI or TDI.

In case of minor intermediates to be further used, sold or fuel gas to be applied in combustion processes in specific production processes, allocation was done according to mass, current market prices or energy. A quantified sensitivity analysis was performed whenever different allocation possibilities were applicable.

In the refinery operations, co-production was addressed by applying allocation based on mass and net calorific value [GaBi 5 2011]. 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 %.

Life Cycle Inventory (LCI) Results

Formats of LCI Dataset

The Eco-profile is provided in three electronic formats:

- As input/output table in Excel®
- As XML document in EcoSpold format (www.ecoinvent.org)
- As XML document in ILCD format (http://lct.jrc.ec.europa.eu)

Key results are summarised below.

Energy Demand

As a key indicator on the inventory level, the **primary energy demand** (system input) of 59.89 MJ/kg TDI and 62.91 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 net calorific value (lower heating value, LHV) is 21.8 MJ/kg TDI and 26.8 MJ/kg MDI.

As a measure of the share of primary energy incorporated in the product, and hence indicating a recovery potential, the **energy content in the isocyanate** (system output), quantified as the gross calorific value (UHV), is 22,4 MJ/kg TDI and 27.6 MJ/kg MDI.

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 isocyanate)	22.40
Process energy (quantified as difference between primary energy demand and energy content of polymer)	37.49
Total primary energy demand	**59.89**

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 isocyanate)	27.60
Process energy (quantified as difference between primary energy demand and energy content of polymer)	35.31
Total primary energy demand	**62.91**

Consequently, the difference (Δ) between primary energy input and energy content in polymer 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 accounted for allocation.

Table 5 and Table 6 show the total energy input (primary energy demand) is used as fuel or feedstock. Fuel use means generating process energy, whereas feedstock use means incorporating hydrocarbon resources into the polymer. Note that some feedstock input may still be valorised as energy; furthermore, process energy requirements may also be affected by exothermal or endothermal reactions of intermediate products. Hence, there is a difference between the feedstock energy input and the energy content of the polymer (measurable as its gross calorific value). Considering this uncertainty of the exact division of the process energy as originating from either fuels or feedstocks, as well as the use of average data (secondary data) in the modelling with different country-specific grades of crude oil and natural gas, the feedstock energy is presented as a range.

Table 5: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1kg TDI

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	2.17	0.08	0.00	1.94
Oil	16.94	0.37	11.4 – 13.4	3.54 – 5.54
Natural gas	32.53	0.67	1.5 – 3.5	29.03 – 31.03
Lignite	1.87	0.14	0.00	1.63
Nuclear	5.07	1.12E-05	0.00	4.84
Biomass	0.00	0.00	0.00	0.00
Hydro	0.40	0.00	0.00	0.38
Solar	0.48	0.00	0.00	0.43
Geothermics	0.00	0.00	0.00	0.00
Waves	0.00	0.00	0.00	0.00
Wood	0.00	0.00	0.00	0.00
Wind	0.43	0.00	0.00	0.38
Other renewable fuels	0.00	0.00	0.00	0.00
Sub-total renewable	**1.32**	**0.00**	**0.00**	**1.32**
Sub-total Non-renewable	**58.57**	**1.26**	**12.9 – 16.9**	**41.67 – 45.67**
Total	**59.89**	**1.26**	**12.9 – 16.9**	**42.99 – 46.99**

Table 6: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1kg MDI

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	2.87	0.10	0.00	2.87
Oil	24.22	0.53	7.2 – 9.2	15.02 – 17.02
Natural gas	29.41	0.60	3.2 – 5.2	24.21 – 26.21
Lignite	1.70	0.13	0.00	1.70
Nuclear	3.40	7.53E-06	0.00	3.40
Biomass	0.00	0.00	0.00	0.00
Hydro	0.31	0.00	0.00	0.31
Solar	0.53	0.00	0.00	0.53
Geothermics	0.01	0.00	0.00	0.01
Waves	0.00	0.00	0.00	0.00
Wood	0.00	0.00	0.00	0.00
Wind	0.48	0.00	0.00	0.48
Other renewable fuels	0.00	0.00	0.00	0.00
Sub-total renewable	**1.32**	**0,00**	**0.00**	**1.32**
Sub-total Non-renewable	**61.59**	**1.37**	**10.40 – 14.40**	**47.20 – 51.20**
Total	**62.91**	**1.37**	**10.40 – 14.40**	**48.52 – 52.52**

Table 7 shows that nearly all of the primary energy demand is from non-renewable resources. Since the scope of ISOPA and their member companies is the isocyanate production, Table 9 and Table 10 analyse the types of useful energy inputs in the polymerisation: electricity has a minor contribution, whereas the majority is thermal energy (heat). This represents the share of the energy requirement that is under operational control of the isocyanate producer (Figure 4). Accordingly, Table 11 and Table 12 show that the majority (81% for TDI and 91% for MDI) of the primary energy demand is accounted for by upstream processes. Finally, Table 13 and Table 14 provide a more detailed overview of the key processes along the production system, their contribution to primary energy demand and how this is sourced from the respective energy resources. This puts the predominant contribution of the production into perspective with the precursors (»other chemicals«). In order to analyse these upstream operations more closely, please refer to the Eco-profiles of the respective precursors. It should be noted, however, that the LCI tables in the annex account for the entire cradle-to-gate primary energy demand of the TDI and MDI system.

Table 7: Primary energy demand by renewability per 1kg TDI

Fuel/energy input type	Value [MJ]	%
Renewable energy resources	1.32	2%
Non-renewable energy resources	58.57	98%
Total	**59.89**	**100%**

Table 8: Primary energy demand by renewability per 1kg MDI

Fuel/energy input type	Value [MJ]	%
Renewable energy resources	1.32	2%
Non-renewable energy resources	61.59	98%
Total	**62.91**	**100%**

Table 9: Analysis by type of useful energy (TDI production – unit process level) per 1kg TDI

Type of useful energy in process input	Value [MJ]
Electricity	1.16
Heat, thermal energy	5.52
Other types of useful energy (relevant contributions to be specified)	
Total (for selected key process)	**6.68**

Table 10: Analysis by type of useful energy (MDI production – unit process level) per 1kg MDI

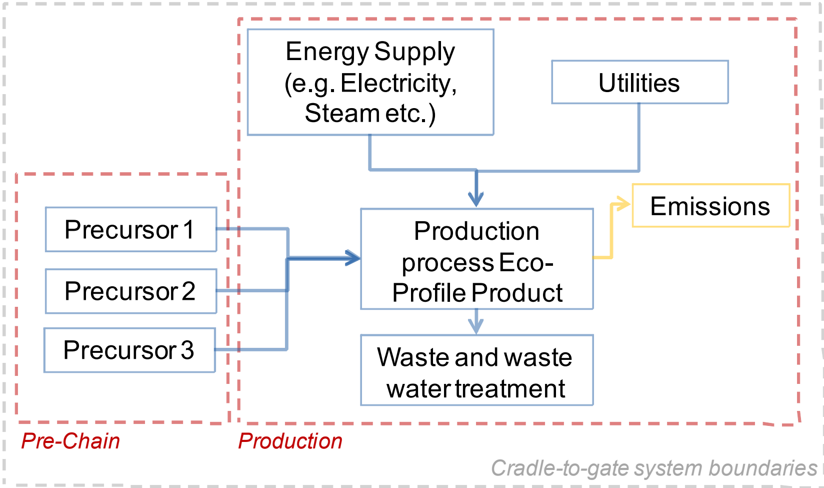
Type of useful energy in process input	Value [MJ]
Electricity	0.72
Heat, thermal energy	3.42
Other types of useful energy (relevant contributions to be specified)	
Total (for selected key process)	**4.15**

Table 11: Contribution to primary energy demand (dominance analysis) per 1kg TDI

Contribution to Primary Energy per segment	Value [MJ]	%
TDI Production (electricity, steam, TDI&TDA unit process, utilities, waste treatment)	11.55	19%
Pre-chain	48.34	81%
Total	**59.89**	**100%**

Table 12: Contribution to primary energy demand (dominance analysis) per 1kg MDI

Contribution to Primary Energy per segment	Value [MJ]	%
MDI Production (electricity, steam, MDI & MDA unit process, utilities, waste treatment)	5.53	9%
Pre-chain	57.38	91%
Total	**62.91**	**100%**



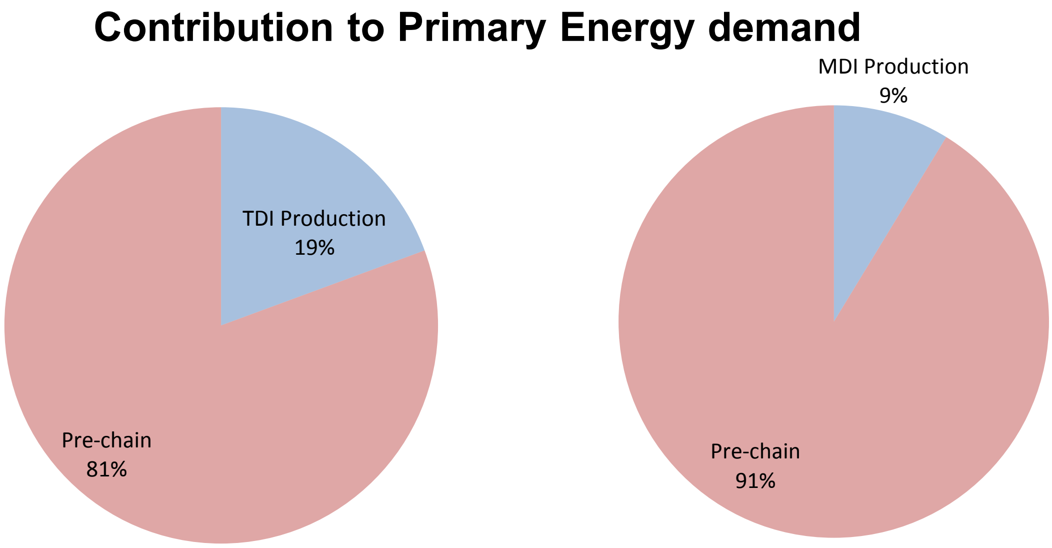


Figure 4: Contribution to primary energy demand per segment

Table 13: Contribution of life cycle stages to total primary energy demand (gross calorific values) per 1kg TDI, see

Total Primary Energy [MJ]	Nitric acid, toluene and TDI process	Other Chemicals	Utilities	Electricity	Thermal Energy	Process Waste Treatment
Coal	0.19	1.59	0.04	0.32	0.02	0.01
Oil	14.81	1.94	0.07	0.07	0.03	0.02
Natural gas	6.47	17.09	0.07	1.06	7.81	0.02
Lignite	0.19	1.28	0.02	0.36	0.01	0.01
Nuclear	0.27	3.47	0.03	1.25	0.04	0.01
Biomass	0.00	0.00	0.00	0.00	0.00	0.00
Hydro	0.03	0.27	0.00	0.10	0.00	0.00
Solar	0.04	0.34	0.01	0.09	0.00	0.00
Geothermics	1.50E-04	5.43E-04	1.15E-04	6.71E-05	5.91E-05	1.00E-05
Waves	0.00	0.00	0.00	0.00	0.00	0.00
Wood	0.00	0.00	0.00	0.00	0.00	0.00
Wind	0.04	0.31	0.01	0.07	0.00	0.00
Other renewable fuels	0.00	0.00	0.00	0.00	0.00	0.00
Total	**22.05**	**26.29**	**0.25**	**3.31**	**7.92**	**0.06**

Table 14: Contribution of life cycle stages to total primary energy demand (gross calorific values) per 1kg MDI, see

Total Primary Energy [MJ]	Aniline and MDI process	Other Chemicals	Utilities	Electricity	Thermal Energy	Process Waste Treatment
Coal	0.34	1.63	0.02	0.37	0.50	0.01
Oil	23.32	0.80	0.01	0.05	0.03	0.01
Natural gas	16.83	8.86	0.03	0.83	2.85	0.01
Lignite	0.27	1.25	0.01	0.16	0.01	0.00
Nuclear	0.61	2.32	0.02	0.43	0.01	0.00
Biomass	0.00	0.00	0.00	0.00	0.00	0.00
Hydro	0.06	0.21	0.00	0.03	0.00	0.00
Solar	0.07	0.39	0.00	0.06	0.00	0.00
Geothermics	1.43E-03	3.60E-03	1.33E-06	1.25E-03	5.34E-05	1.50E-06
Waves	0.00	0.00	0.00	0.00	0.00	0.00
Wood	0.00	0.00	0.00	0.00	0.00	0.00
Wind	6.41E-02	3.54E-01	3.63E-03	5.25E-02	1.02E-03	7.34E-04
Other renewable fuels	0.00	0.00	0.00	0.00	0.00	0.00
Total	**41.58**	**15.81**	**0.10**	**1.99**	**3.39**	**0.04**

Water Consumption

Table 15: Gross water resources table per 1kg TDI

Source	Process water [kg]	Cooling water [kg]	Total [kg]
Public supply	–	–	–
River/canal	1.9	15.1	17.0
Sea	0.6	–	0.6
Unspecified	0.6	–	0.6
Well	–	–	–
Totals	**3.1**	**15.1**	**18.2**

Table 16: Gross water resources table per 1kg MDI

Source	Process water [kg]	Cooling water [kg]	Total [kg]
Public supply	–	–	–
River/canal	1.6	19.0	20.6
Sea	0.8	–	0.8
Unspecified	0.6	–	0.6
Well	–	–	–
Totals	**3.0**	**19.0**	**22.0**

Air Emission Data

Table 17 and Table 18 show a few selected air emissions which are commonly reported and used as key performance indicators; for a full inventory of air emissions, please refer to the complete LCI table in the annex of this report.

Table 17: Selected air emissions per 1kg TDI

Air emissions	kg
Carbon dioxide, fossil (CO_2, fossil)	2.14
Carbon monoxide (CO)	1.22E-03
Sulphur dioxide (SO_2)	1.82E-03
Nitrogen oxides (NO_x)	3.04E-03
Particulate matter ≤ 10 µm (PM 10)	7.69E-05

Table 18: Selected air emissions per 1kg MDI

Air emissions	kg
Carbon dioxide, fossil (CO_2, fossil)	2.04
Carbon monoxide (CO)	1.20E-03
Sulphur dioxide (SO_2)	2.12E-03
Nitrogen oxides (NO_x)	3.18E-03
Particulate matter ≤ 10 µm (PM 10)	5.51E-05

Wastewater Emissions

Table 19 and Table 20 show a few selected wastewater emissions which are commonly reported and used as key performance indicators; for a full inventory of wastewater emissions, please refer to the complete LCI table in the annex of this report.

Table 19: Selected water emissions per 1kg TDI

Water emissions	kg
Biological oxygen demand after 5 days (BOD 5)	3.21E-05
Chemical oxygen demand (COD)	2.44E-04
Total organic carbon (TOC)	8.84E-06

Table 20: Selected water emissions per 1kg MDI

Water emissions	kg
Biological oxygen demand after 5 days (BOD 5)	3.05E-05
Chemical oxygen demand (COD)	2.97E-04
Total organic carbon (TOC)	1.25E-05

Solid Waste

Table 21: Solid waste generation per 1kg TDI (key foreground process level)

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous	_	_	8.04E-05	_	8.04E-05
Hazardous	3.17E-02	_	_	_	3.17E-02
Unspecified	_	_	_	_	_
Total	3.17E-02	_	8.04E-05	_	3.18E-02

Table 22: Solid waste generation per 1kg MDI (key foreground process level)

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous	5.97E-03	_	2.64E-05	_	6.00E-03
Hazardous	8.97E-04	_	_	_	8.97E-04
Unspecified	_	_	_	_	_
Total	6.87E-03	_	2.64E-05	_	6.89E-03

Life Cycle Impact Assessment

Input

Natural Resources

Table 23: Abiotic Depletion Potential per 1kg TDI

Natural resources	Value
Abiotic Depletion Potential (ADP). elements [kg Sb eq]	6.67E-06
Abiotic Depletion Potential (ADP). fossil fuels [MJ]	48.90

Table 24: Abiotic Depletion Potential per 1kg MDI

Natural resources	Value
Abiotic Depletion Potential (ADP). elements [kg Sb eq]	6.04E-06
Abiotic Depletion Potential (ADP). fossil fuels [MJ]	53.42

Please note that differences between the primary energy demand and the "Abiotic Depletion Potential (ADP), fossil fuels" can be expected, as the latter considers the net calorific value on average whereas the primary energy demand presented in this report refers to the gross calorific value and considers country-specific resources.

Output

Climate Change

Table 25: Global Warming Potential (100 years) per 1kg TDI

Climate change	kg CO_2 eq.
Global Warming Potential (GWP)	2.71

Table 26: Global Warming Potential (100 years) per 1kg MDI

Climate change	kg CO_2 eq.
Global Warming Potential (GWP)	2.39

Acidification

Table 27: Acidification Potential per 1kg TDI

Acidification of soils and water bodies	g SO_2 eq.
Acidification Potential (AP)	3.87

Table 28: Acidification Potential per 1kg MDI

Acidification of soils and water bodies	g SO_2 eq.
Acidification Potential (AP)	4.30

Eutrophication

Table 29: Eutrophication Potential per 1kg TDI

Eutrophication of soils and water bodies	g PO_4^{3-} eq.
Eutrophication Potential (EP), total	0.87

Table 30: Eutrophication Potential per 1kg MDI

Eutrophication of soils and water bodies	g PO_4^{3-} eq.
Eutrophication Potential (EP), total	0.68

Ozone Depletion

Table 31: Ozone Depletion Potential per 1kg TDI

	g CFC-11 eq.
Ozone Depletion Potential (ODP)	6.65E-05

Table 32: Ozone Depletion Potential per 1kg MDI

	g CFC-11 eq.
Ozone Depletion Potential (ODP)	7.69E-03

Summer Smog

Table 33: Photochemical Ozone Creation Potential per 1kg TDI

	g Ethene eq.
Photochemical Ozone Creation Potential	0.64

Table 34: Photochemical Ozone Creation Potential per 1kg MDI

	g Ethene eq.
Photochemical Ozone Creation Potential	0.68

Dust & Particulate Matter

Table 35: PM10 emissions per 1kg TDI

Particulate matter	g PM10 eq.
Particulate matter ≤ 10 µm. total	0.077
Particulate matter ≤ 10 µm (direct emissions)	–
Particulate matter ≤ 10 µm. secondary	0.077

Table 36: PM10 emissions per 1kg MDI

Particulate matter	g PM10 eq.
Particulate matter ≤ 10 µm. total	0.055
Particulate matter ≤ 10 µm (direct emissions)	–
Particulate matter ≤ 10 µm. secondary	0.055

Dominance Analysis

Table 37 and Table 38 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.

Regarding TDI in all analysed environmental impact categories, intermediates contribute to about 80 % or more of the total impact, with a balanced share between its main intermediates nitric acid and toluene and other chemicals.

Regarding MDI in all analysed environmental impact categories, intermediates contribute to about 90 % or more of the total impact, with aniline dominating with about 60 % or more (the only exception being the indicator ADP Elements). The use of high quality data especially for this case is therefore decisive to the environmental profile of MDI.

Table 37: Dominance analysis of impacts per 1kg TDI

	Total Primary Energy [MJ]	ADP Elements [kg Sb eq.]	ADP Fossil [MJ]	GWP [kg CO_2 eq.]	AP [g SO_2 eq.]	EP [g PO_4^{3-} eq]	POCP [g Ethene eq.]
Nitric acid, toluene and TDI process	37.2%	2.1%	41.4%	36.0%	37.9%	62.7%	47.0%
Other chemicals	43.5%	96.7%	40.3%	40.4%	45.0%	26.2%	38.9%
Utilities	0.4%	0.6%	0.4%	0.7%	0.9%	0.8%	0.8%
Electricity	5.5%	0.2%	3.4%	4.9%	6.4%	2.7%	3.3%
Thermal Energy	13.2%	0.3%	14.5%	16.1%	9.2%	6.5%	9.7%
Process waste treatment	0.1%	0.07%	0.10%	1.9%	0.6%	1.2%	0.3%
Total	100%	100%	100%	100%	100%	100%	100%

Table 38: Dominance analysis of impacts per 1kg MDI

	Total Primary Energy [MJ]	ADP Elements [kg Sb eq.]	ADP Fossil [MJ]	GWP [kg CO_2 eq.]	AP [g SO_2 eq.]	EP [g PO_4^{3-} eq]	POCP [g Ethene eq.]
Aniline and MDI process	66.1%	5.8%	70.3%	58.8%	59.2%	65.2%	71.4%
Other chemicals	25.1%	93.4%	21.4%	27.6%	31.0%	26.7%	22.0%
Utilities	0.2%	0.4%	0.1%	0.2%	0.2%	0.2%	0.1%
Electricity	3.2%	0.1%	2.4%	4.3%	4.9%	2.8%	2.6%
Thermal Energy	5.4%	0.1%	5.8%	8.6%	4.4%	4.1%	3.7%
Process waste treatment	0.1%	0.09%	0.06%	0.5%	0.3%	1.0%	0.2%
Total	100%	100%	100%	100%	100%	100%	100%

Comparison of the present Eco-profile with its previous version (2005)

As discussed in the section Allocation Rules, the results for both TDI and MDI depend substantially on the chosen allocation procedure. In the previous version of this Eco-profile, however, the adopted allocation method had not been documented. Hence, a direct comparison of the results published in this Eco-profile and the previous version is not possible. The current version transparently sets out what is held to be the best available state of knowledge on this subject.

Table 39: Comparison of the present TDI Eco-profile with its previous version (2005)

Environmental Impact Categories	Eco-profile TDI (2005)	Eco-profile TDI (2011)	Comment
Gross primary energy from resources [MJ]	108.05	58.57	
Abiotic Depletion Potential (ADP), elements [kg Sb eq.]	7.36E-06	6.67E-06	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	89.69	48.90	These results are not
Global Warming Potential (GWP) [kg CO_2 eq.]	6.36	2.71	comparable. Please
Acidification Potential (AP) [g SO_2 eq.]	30.66	3.87	see comment above.
Eutrophication Potential (EP) [g PO_4^{3-} eq.]	4.24	0.87	
Ozone Depletion Potential (ODP) [g CFC-11 eq.]	0	6.65E-05	
Photochemical Ozone Creation Potential [g Ethene eq.]	2.53	0.64	

Table 40: Comparison of the present MDI Eco-profile with its previous version (2005)

Environmental Impact Categories	Eco-profile MDI (2005)	Eco-profile MDI (2011)	Comment
Gross primary energy from resources [MJ]	94.88	61.59	
Abiotic Depletion Potential (ADP), elements [kg Sb eq.]	9.41E-06	6.04E-06	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	80.72	53.42	These results are not
Global Warming Potential (GWP) [kg CO_2 eq.]	4.02	2.39	comparable. Please
Acidification Potential (AP) [g SO_2 eq.]	17.11	4.30	see comment above.
Eutrophication Potential (EP) [g PO_4^{3-} eq.]	1.36	0.68	
Ozone Depletion Potential (ODP) [g CFC-11 eq.]	0.000000	7.69E-03	
Photochemical Ozone Creation Potential [g Ethene eq.]	1.44	0.68	

Review

Review Details

The project included regular milestone meetings with representatives of all participating producers and PlasticsEurope as system operator. The reviewer participated in these meetings. In addition, a review meeting between the LCA practitioner and the reviewer was held, including a model and database review, and spot checks of data and calculations.

Review Summary

The LCA practitioner has demonstrated a very good competence and experience, with a track record of LCA projects in the chemical and plastics industry. A dominance analysis was conducted to identify sensitive data requirements prior to the data collection. Original data were collected for all foreground processes, while background process data were taken from the GaBi database which is likewise of good quality[2].

For TDI the precursors nitric acid and toluene, for MDI the precursor aniline, were shown to have the most substantial influence on the results. Although the precision of the dataset was not formally calculated by means of a statistical analysis, it is assessed to be very good for two reasons: first, because of the clear procedure adopted, and second, because of the robustness achieved by being based upon an average of different discrete European production sites. The sites were individually analysed and specifically modelled, representing the respective technologies. The deviation among the degree of detail and consistency was found to be low.

For the by-product HCl (100%), mass allocation was applied, following a conservative approach and reflecting the purpose of the operations.

Calculation and reporting were subject to extensive analysis and review. As a result, this dataset is assessed to be a reliable and high-quality representation of TDI and MDI production in Europe.

Reviewer Name and Institution

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[2] The results reported in this Eco-profile are determined by the original data collected for all foreground processes. In view of the dominance analysis, the use of generic datasets from the GaBi 5 database is not considered to have a substantial influence on the results. As the GaBi 5 database is well documented and good quality, this choice is deemed appropriate and reproducible.

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2012-04

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