Aliphatic Isocyanates for Polyurethane Products
ALIPA

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

December 2014

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ALIPA
EUROPEAN ALIPHATIC ISOCYANATES PRODUCERS ASSOCIATION

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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 judgment between environmental criteria.

This EPD describes the production of aliphatic isocyanates from cradle to gate (from crude oil extraction to liquid at plant, i.e. aliphatic isocyanate production site output). **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. 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	ALIPA
LCA Practitioner	PE INTERNATIONAL AG
Programme Owner	PlasticsEurope AISBL
Programme Manager, Reviewer	DEKRA Consulting GmbH
Number of plants included in data collection	5 aliphatic isocyanates; 1 plant per product
Representativeness	Typical representative technology
Reference year	2010
Year of data collection and calculation	2012/2013
Expected temporal validity	2020
Cut-offs	No significant cut-offs
Data Quality	Good
Allocation method	Economic allocation (in foreground system)

Description of the Product and the Production Process

This EPD is for three aliphatic diisocyanate monomers, hexamethylene diisocyanate (HDI), isophorone diisocyanate (IPDI) and hydrogenated methylenediphenyl diisocyanate (H12MDI), and for the homologeous oligomers, hexamethylene diisocyanate trimer (HDI trimer) and isophorone diisocyanate trimer (IPDI trimer), which are predominantly used in the production of isocyanate hardeners for polyurethane coatings.

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.

Aliphatic diisocyanate monomers and their homologous oligomers are mainly used for lightfast, weatherproof and high-quality automotive and industrial coatings.

The reference flows, to which all data given in this EPD refer, is 1 kg of aliphatic isocyanate or corresponding oligomer.

Production Process

The aliphatic diisocyanate monomers HDI and IPDI are made from corresponding diamines by treatment with phosgene. The diamines stem from building blocks, such as butadiene, acetone and phenol.

H12MDI is produced via the urea route (reaction of Bis(para-aminocyclohexyl)methane (PACM) with urea).

In the production of homologeous oligomers of aliphatic diisocyanate, e.g. HDI trimer or IPDI trimer, monomeric diisocyanate is converted in oligomers by catalytic reaction. In a second step residual monomers are removed by a multi-stage distillation.

Data Sources and Allocation

The main data source for the average dataset was a primary data collection from European producers of HDI, IPDI, HDI-trimer, IPDI-trimer and H12MDI. Data of each aliphatic isocyanate are represented by the typical technological process chain. For each product one set of data has been provided. The participating companies represent about 80% of the European production capacity for the considered products. The data for the upstream supply chain and all relevant background data, such as energy and auxiliary materials are taken from the data base of the software system GaBi 5 [GaBi 5 2011].

Use Phase and End-of-Life Management

High quality polyurethane coatings help to preserve resources. They ensure effective protection of a substrate against corrosion, deterioration and mechanical damage and prolong the service life of goods like vehicles, industrial plants and buildings.

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.

Polyurethane coatings or adhesives are typically not separated in the end-of-life stage, but undergo the same procedure as the substrate.

Environmental Performance

The tables below show the environmental performance indicators associated with the production of 1 kg of aliphatic isocyanates.

Input Parameters

Indicator	Unit	Value
Non-renewable energy resources[1]	MJ	141.8
• Fuel energy	MJ	107.5
• Feedstock energy	MJ	34.3
Renewable energy resources (biomass)[1]	MJ	3.2
• Fuel energy	MJ	3.2
• Feedstock energy	MJ	0
Abiotic Depletion Potential		
• Elements	kg Sb eq	9.3E-06
• Fossil fuels	MJ	124.0
Renewable materials (biomass)	kg	0.0
Water use (key foreground process level)	kg	
• total input	kg	3444.5
• total consumption	kg	28.4

[1] Calculated as upper heating value (UHV)

Output Parameters

Indicator	Unit	Value
GWP	kg CO_2 eq	6.5
ODP	g CFC-11 eq	2.1E-05
AP	g SO_2 eq	9.8
POCP	g Ethene eq	2.2
EP	g PO_4 eq	1.6
Dust/particulate matter[2]	g PM10	3.2E-01
Total particulate matter[2]	g	4.4E-01
Waste	kg	1.3E-01
• Radioactive waste	kg	2.4E-03
• Non-radioactive waste [3]	kg	1.3E-01

[2] Including secondary PM10

[3] Non-radioactive wastes include: spoil, tailings, and waste, deposited

Additional Environmental and Health Information

The manufacturers of aliphatic diisocyanate monomers and their homologous oligomers are working through ALIPA to promote Product Stewardship and responsible practice in the value chain. The program "ALIPA Safeguard – We care that you care" provides safe handling information and training materials in many languages.

Additional Technical Information

Aliphatic diisocyanate monomers and their homologous oligomers are primarily used as raw materials for polyurethane coatings, but also for adhesives, sealants, elastomers and other applications.

Additional Economic Information

The main benefits of these polyurethane materials are outstanding adhesion, weather and corrosion resistance, elasticity and flexibility.
Polyurethane based on aliphatic isocyanates show exceptional durability and UV-light stability, chemical and mechanical performances which could not be achieved otherwise.

Information

Data Owner

European Aliphatic Isocyanates Producers Association (ALIPA)
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Programme Manager & Reviewer

DEKRA Consulting GmbH

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

Registration number: PlasticsEurope 2014-003, validation expires on 31 December 2017 (date of next revalidation review).

Programme Owner

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

References

- Cover image with kind permission by ALIPA.
- PlasticsEurope: Eco-profiles and environmental declarations – LCI methodology and PCR for uncompounded polymer resins and reactive polymer precursor (version 2.0, April 2011).

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Goal & Scope

Intended Use & 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 is 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 aliphatic isocyanates (without packaging) »at gate« (production site output) representing a European industry production average.

Product and Producer Description

Product Description

Aliphatic diisocyanate monomers are predominantly used in the production of isocyanate hardeners for polyurethane coatings.

Hexamethylene diisocyanate (HDI) (1,6-diisocyanatohexane)

- CAS no. 822-06-0
- chemical formula: $C_8H_{12}N_2O_2$
- gross calorific value of ca. 30 MJ/kg

Isophorone diisocyanate (IPDI) (5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethyl-cyclohexane)

- CAS no. 4098-71-9
- chemical formula: $C_{12}H_{18}N_2O_2$
- gross calorific value of 31.4 MJ/kg

Dicyclohexylmethane-diisocyanate (H12MDI) (4,4'-Methylenebis(cyclohexyl isocyanate 1-isocyanato-4-[(4-isocyanatohexyl)methyl] hexane)

- CAS no. 5124-30-1
- chemical formula: $C_{15}H_{22}N_2O_2$
- gross calorific value of 33.1 MJ/kg

HDI trimer (1,3,5-tris(6-isocyanatohexyl)-1,3,5-triazinane-2,4,6-trione)

- CAS no. 3779-63-3
- chemical formula: $C_{24}H_{36}N_6O_6$
- gross calorific value of ca. 30 MJ/kg

IPDI trimer (3-Isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate homopolymer)

- CAS no. 53380-05-0
- chemical formula: $C_{36}H_{54}N_6O_6$
- gross calorific value of 31.4 MJ/kg

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

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. Data for this Eco-profile and EPD have been provided by member companies of the European Aliphatic Isocyanates Producers Association (ALIPA).

Life Cycle Inventory

System Boundaries

PlasticsEurope Eco-profiles and EPDs refer to the production of polymers as a cradle-to-gate system (Figure 1).

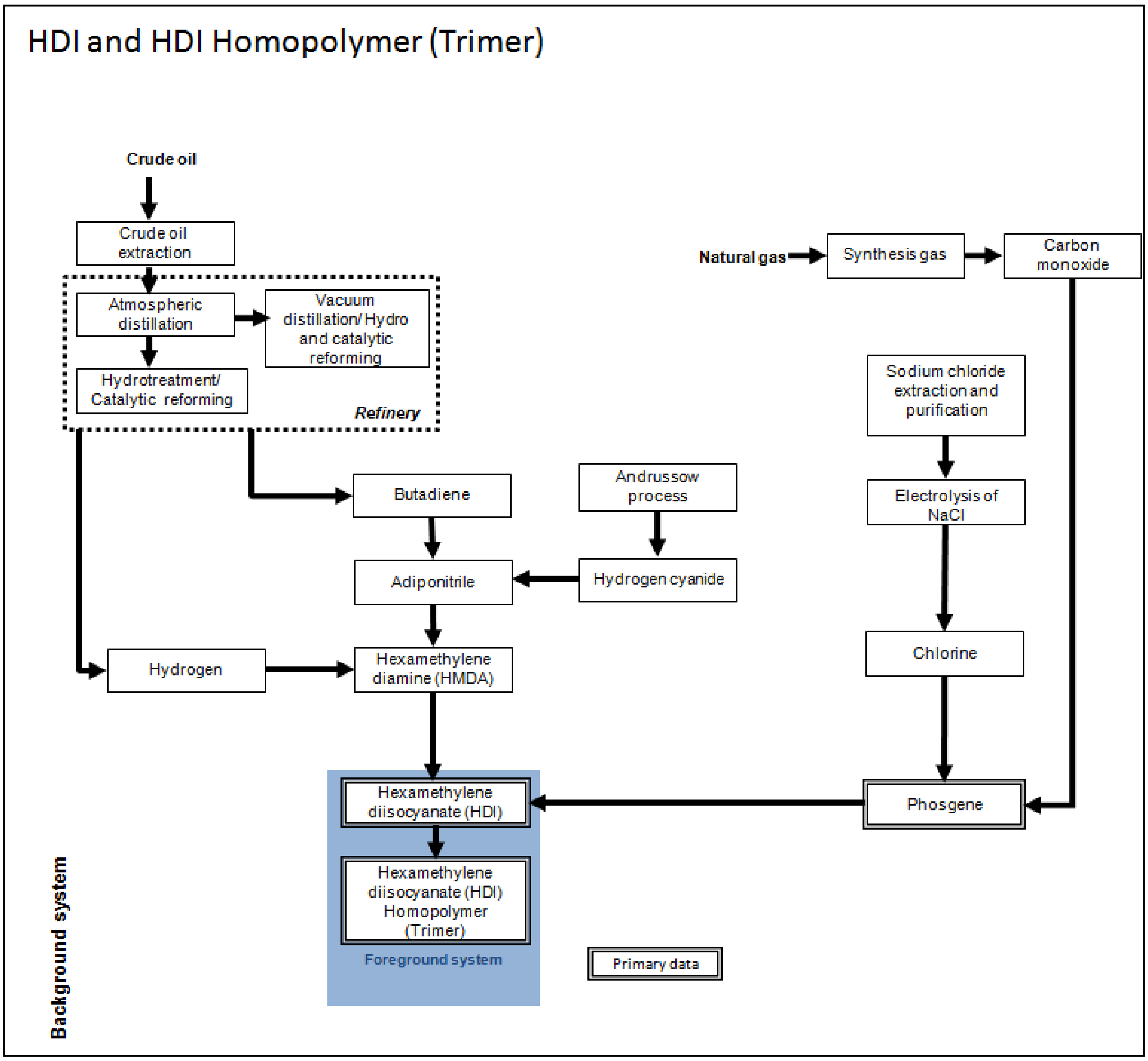


Figure 1: Cradle-to-gate system boundaries (HDI / HDI trimer)

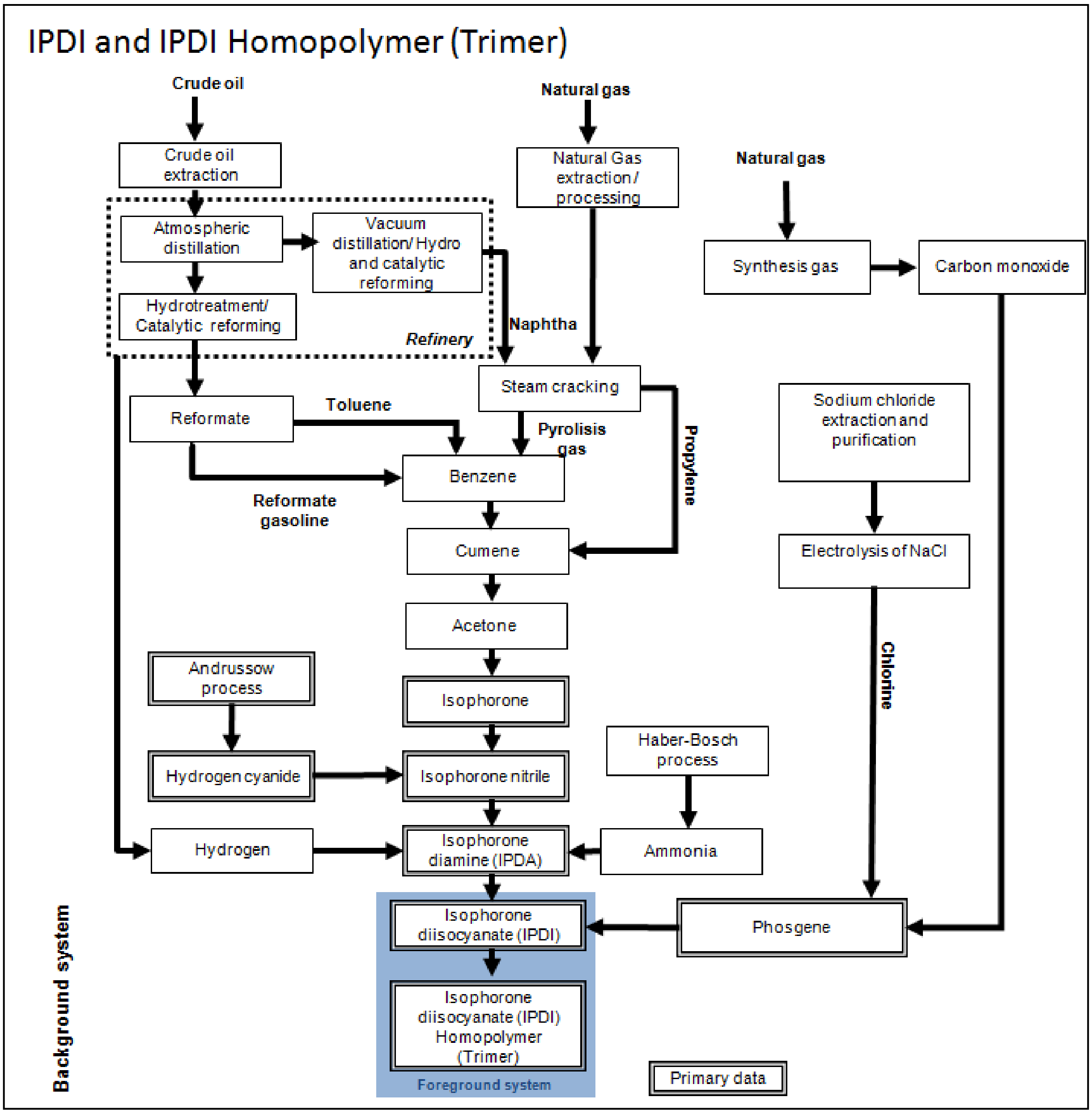


Figure 2: Cradle-to-gate system boundaries (IPDI / IPDI trimer)

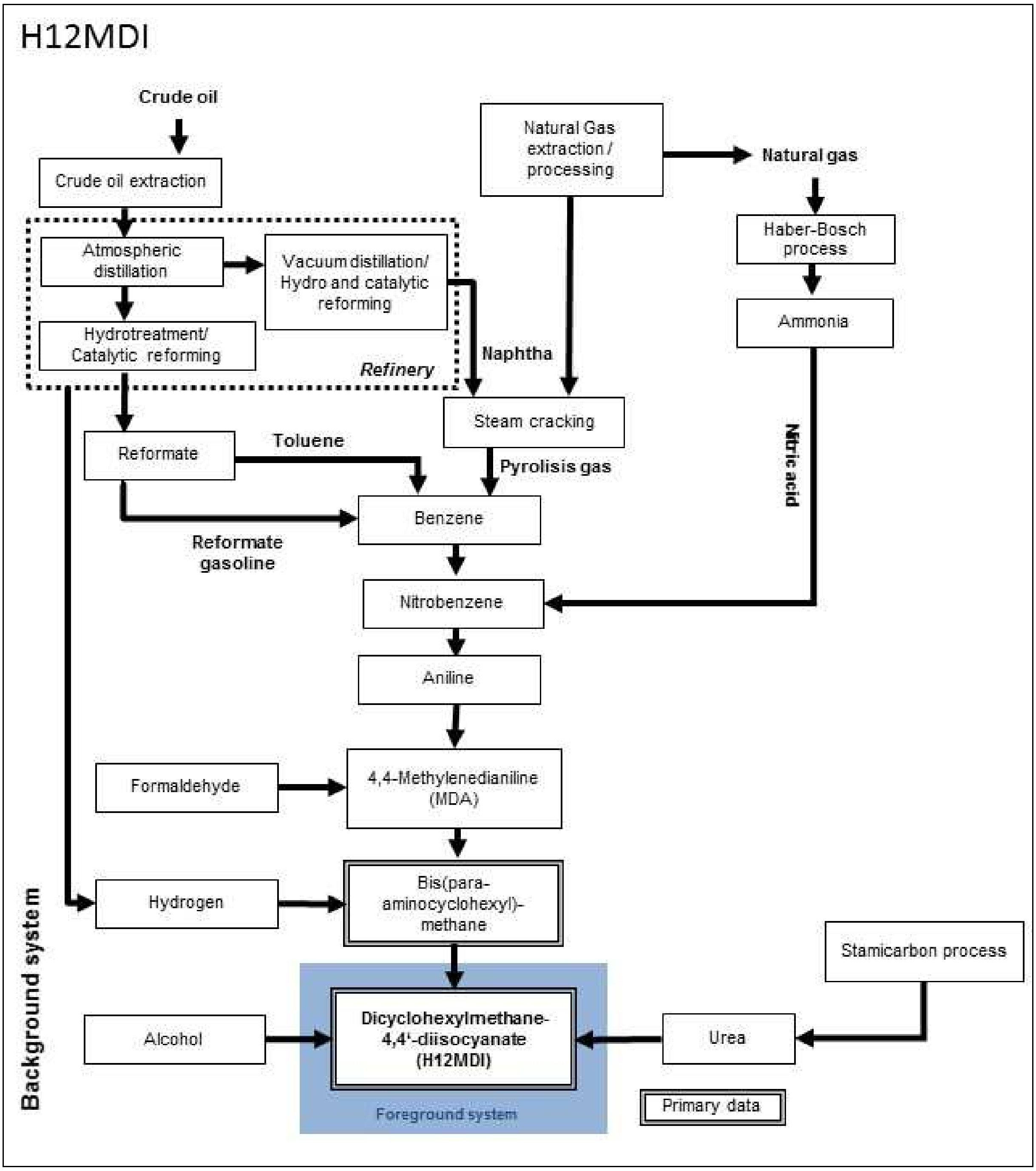


Figure 3: *Cradle-to-gate system boundaries (H12MDI)*

Technological Reference

The production processes were modelled using specific values from primary data collection at site. Each type of aliphatic isocyanate represents the typical technology and processing applied in Europe. The declared products cover more than 80% of the total European aliphatic isocyanates production (EU-27) in 2010.

Primary data were used for all foreground processes (under operational control) complemented with secondary data for background processes (under indirect management control). The data for the upstream supply chain are taken from the database of the software system GaBi 5 [GaBi 5 2011].

For each of the considered five aliphatic isocyanates a software model is generated and represents the applied technological route per isocyanate. The values declared in this Eco-profile for the average aliphatic isocyanate result from the arithmetic average of the five considered products.

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 between 2010 and 2008 for electricity and thermal energy processes. The dataset is considered to be valid until substantial technological changes in the production chain occur. The overall reference year for this Eco-profile is 2010 with a maximal temporal validity until 2020 for the foreground system.

Geographical Reference

Primary production data for the isocyanate production are from two different suppliers in the EU. Whenever applicable (in the majority of the cases), site-specific conditions were applied. Only in cases where no further information was available, average European conditions were used for fuel and energy inputs in the system. 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. Aliphatic isocyanates imported into Europe were not considered in this Eco-profile.

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 unit process and supply chain, (<0.1% by weight of product output) were neglected. In such cases, it was assured that no hazardous substances or metals were present in this neglected part.

According to the GaBi database 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 2% on the total is expected.

Transport processes are included for the relevant material flows.

Data Quality Requirements

Data Sources

Eco-profile and EPDs developed by PlasticsEurope 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 ALIPA (see Producer Description).

All relevant background data such as energy and auxiliary material are taken from the GaBi 5 database [GaBi 5 2011]. Most of the background datasets used are publicly available and documented.

The background data deliver main information for the intermediate product LCIs. The data source for the basic materials' LCIs depends on the specific isocyanate. Figure 1, Figure 2, and Figure 3 display more details and show the degree of primary data and background data. The impact of the supply chain, i.e. the basic materials contributes to more than 88% of the overall impact (Table 20).

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 from the most important producers in Europe in order to generate a European industry average production. The environmental contributions of each process to the overall LCI results are described in the Chapter 'Life Cycle Impact Assessment'.

Representativeness

The participating companies represent 80% of the European aliphatic isocyanate production in 2010. The selected background data can be regarded as representative for the intended purpose.

Consistency

To ensure consistency only primary data of the same level of detail and background data from the GaBi 5 databases 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. In addition to the external review, an internal independent quality check was performed (see 'Internal Independent Quality Assurance Statement').

Reliability

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 aliphatic isocyanate covers all related flows in accordance with the above cut-off criteria. In this way all relevant flows were quantified and data is considered complete. Waste treatment was included in the model, so that only elementary flows cross the system boundaries.

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. The generation of a technology average leads to a systematic bandwidth of the results.

Reproducibility

Reproducibility is given for internal use since the owners of the technologies provided the data under confidentiality agreements. 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 5 software [GaBi 5 2011]. 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.

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 database is updated regularly and continuously validated.

Life Cycle Model

The study has been performed with the LCA software GaBi 5 [GaBi 5 2011]. The associated database integrates ISO 14040/44 requirements. Due to confidentiality reasons details on software modelling and methods used cannot be shown here. However, provided that appropriate confidentiality agreements are in place the model can be reviewed in detail; an external independent review was conducted to this aim. 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 4).

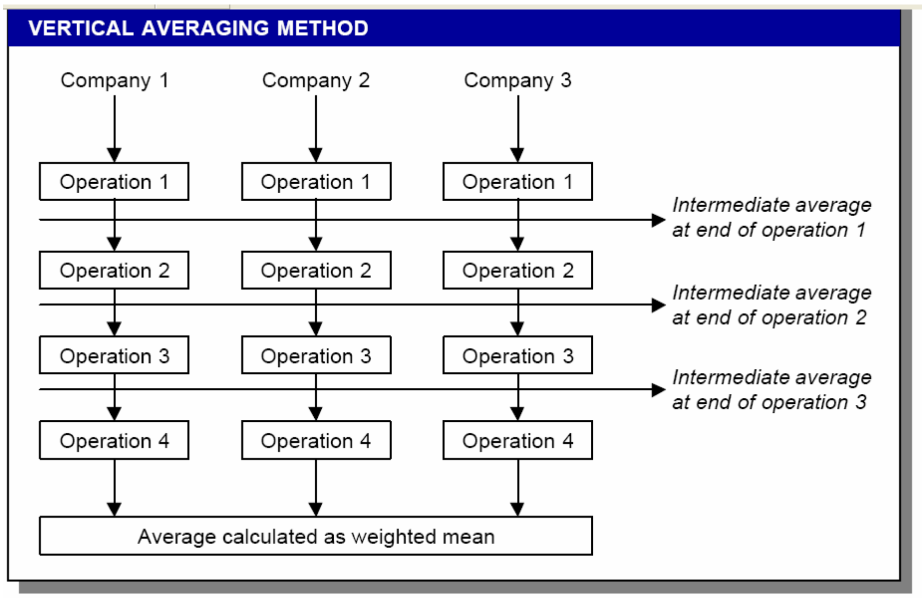


Figure 4: *Vertical Averaging (source: Eco-profile of high volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001)*

The production methods for the five isocyanates as well as the basic materials differ. This results in higher bandwidth. The deviation of the single products regarding the results of the considered impact categories in reference to the average values are up to -90% / +110% . This is especially due to the very low absolute values for the categories ozone depletion potential (ODP) and abiotic depletion potential - elements (ADP), where small changes in the results have a big impact on the range; hence, the values are still displaying the same order of magnitude.

Due to confidentiality reasons, the average of the five aliphatic isocyanates follows an arithmetic approach, which directly forwards the bandwidth in the average result. For the application of the data this needs to be considered.

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 do not exist or alternative technologies show complete 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.

Foreground system

The production processes for the aliphatic isocyanates HDI and IPDI deliver hydrogen chloride as co-product. As the produced hydrogen chloride is sold and the economic value of the products differ significantly, an economic allocation has been applied in the software model.

Background system

In the refinery operations, co-production was addressed by applying allocation based on mass and net calorific value [GaBi 5 2011]. The manufacturing route of every refinery product is modelled and so the effort of the production of these products is calculated specifically. Two allocation rules are applied: 1. the raw material (crude oil) consumption of the respective stages, which is necessary for the production of a product or an intermediate product, is allocated by energy (mass of the product * calorific value of the product); and 2. the energy consumption (thermal energy, steam, electricity) of a process, e.g. atmospheric distillation, being required by a product or an intermediate product, are charged on the product according to the share of the throughput of the stage (mass allocation).

Materials and chemicals needed during manufacturing are modelled using the allocation rule most suitable for the respective product. For further information on a specific product see documentation.gabi-software.com

For the generation of life cycle inventories for electrical and thermal energy beside above mentioned allocation methods for refinery products and materials allocations by economic value are applied, dependent on the specific technique. In case of plants for the co-generation of heat and power allocations by exergy are applied.

The chosen allocation in refinery is based on several sensitivity analyses, which was reviewed by petrochemical experts. The relevance and influence of different possible allocation keys in this context is small. In steam cracking, allocation according to net calorific value with regard to the whole product range was applied. The difference compared with mass allocation is below 2%.

In the supply chain of single aliphatic isocyanates price allocation was applied as the co-products are marketable.

Life Cycle Inventory (LCI) Results

Formats of LCI Dataset

The Eco-profile is provided in four 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)
- As GBX file in GaBi format (www.gabi-software.com)

Key results are summarised below.

Energy Demand

As a key indicator on the inventory level, the **primary energy demand** (system input) of 145.0 MJ/kg 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).

As a measure of the share of primary energy incorporated in the product, and hence indicating a recovery potential, the **energy content in the polymer** (system output), quantified as the gross calorific value (UHV), is 31.18 MJ/kg.

Table 1: Primary energy demand (system boundary level) per 1kg aliphatic isocyanate

Primary Energy Demand	Value [MJ]
Energy content in polymer (energy recovery potential, quantified as gross calorific value)	31.2
Process energy (quantified as difference between primary energy demand and energy content)	113.8
Total primary energy demand	**145.0**

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 removed during allocation.

Table 2 shows how 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 exothermic or endothermic 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 approximate data.

Table 2: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1kg aliphatic isocyanate

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	8.2	0.3	0.0	8.2
Oil	35.7	0.8	ca. 10.4	ca. 25.6
Natural gas	86.2	1.8	ca. 24.3	ca. 62.0
Lignite	5.7	0.4	0.0	5.7
Nuclear	5.95	1.32E-05	0.0	5.9
Biomass	0.0	0.0	0.0	0.0
Hydro	0.7	0.0	0.0	0.7
Solar	1.3	0.0	0.0	1.3
Geothermics	0.0	0.0	0.0	0.0
Waves	0.0	0.0	0.0	0.0
Wood	0.0	0.0	0.0	0.0
Wind	1.3	0.0	0.0	1.3
Other renewable fuels	0.0	0.0	0.0	0.0
Sub-total renewable	**3.2**	**0**	**0**	**3.2**
Sub-total Non-renewable	**141.8**	**3.3**	**ca. 34.7**	**ca. 107.5**
Total	**145.0**	**3.3**	**ca. 34.7**	**ca. 110.7**

Table 3 shows that nearly all of the primary energy demand is from non-renewable resources. Since the scope of PlasticsEurope and their member companies is the polymer and precursor production, Table 4 analyses the types of useful energy inputs in the last step of the isocyanate production: electricity has a minor contribution, whereas the majority is thermal energy (heat) (considered as direct energy value without conversion to primary energy). This represents the share of the energy requirement that is under operational control of the isocyanate producer (Figure 5).

Accordingly, Table 5 shows that the majority (94%) of the primary energy demand is accounted for by upstream processes. Finally, Table 6 provides 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. It should be noted, however, that the LCI tables in the annex account for the entire cradle-to-gate primary energy demand of the aliphatic isocyanate system.

Table 3: Primary energy demand by renewability per 1kg aliphatic isocyanate

Fuel/energy input type	Value [MJ]	%
Renewable energy resources	3.2	2
Non-renewable energy resources	141.8	98
Total	**145.0**	**100**

Table 4: Analysis by type of useful energy (production – unit process level) per 1kg aliphatic isocyanate

Type of useful energy in process input	Value [MJ]
Electricity	1.2
Heat, thermal energy	4.9
Other types of useful energy (relevant contributions to be specified)	0.1*
Total (for selected key process)	6.2

*Electrical energy for compressed air and cooling cycle

Table 5: Contribution to primary energy demand (dominance analysis) per 1kg aliphatic isocyanate

Contribution to Primary Energy per segment	Value [MJ]	%
Production (electricity, thermal energy, unit process, utilities, transport, waste treatment)	9.0	6
Pre-chain	136.0	94
Total	**145.0**	**100**

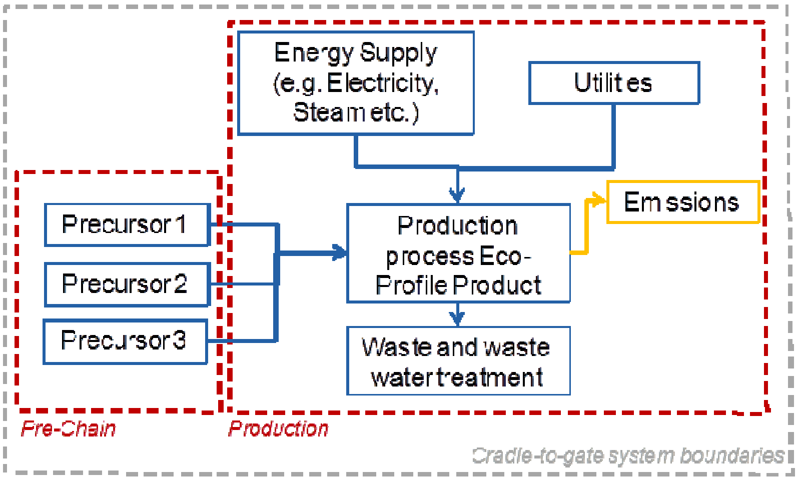
The column basic material and process in Table 6 displays the primary energy demand of the supply chain of the main input material of the respective unit process of each isocyanate. Other chemicals are additional substances declared by the participants of the study, but used in minor amounts. The column utilities covers the primary energy demand necessary for water conditioning and inert gas (nitrogen).

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

Total Primary Energy [MJ]	Precursors and process*	Other Chemicals	Utilities**	Electricity	Thermal Energy	Transport	Process Waste Treatment
Coal	6.2	4.5E-02	1.7E-02	1.6E+00	3.0E-01	4.4E-03	2.3E-03
Oil	34.9	4.9E-01	7.6E-03	9.7E-02	3.8E-02	9.9E-02	5.9E-03
Natural gas	80.8	5.6E-01	1.6E-02	3.6E-01	4.5E+00	1.3E-02	5.8E-03
Lignite	4.9	1.2E-02	2.0E-02	6.5E-01	1.1E-01	3.2E-03	1.1E-03
Nuclear	5.2	2.2E-02	1.8E-02	5.8E-01	9.9E-02	6.4E-03	1.0E-03
Biomass	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Hydro	0.6	3.7E-03	1.9E-03	6.2E-02	1.1E-02	1.2E-03	1.3E-04
Solar	1.1	3.4E-03	4.3E-03	1.4E-01	2.5E-02	4.5E-03	2.4E-04
Geothermics	6.8E-03	4.6E-04	8.2E-07	5.2E-06	4.3E-06	5.9E-05	1.2E-06
Waves	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wood	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Wind	1.1	2.9E-03	4.2E-03	1.4E-01	2.4E-02	8.3E-04	2.2E-04
Other renewable fuels	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total	**134.9**	**1.1**	**0.1**	**3.7**	**5.1**	**0.1**	**0.0**

* Precursors and process include diamines, phosgene, urea, PACM, and direct process emissions

** Utilities include e.g. inert gases, compressed air, process water, etc.



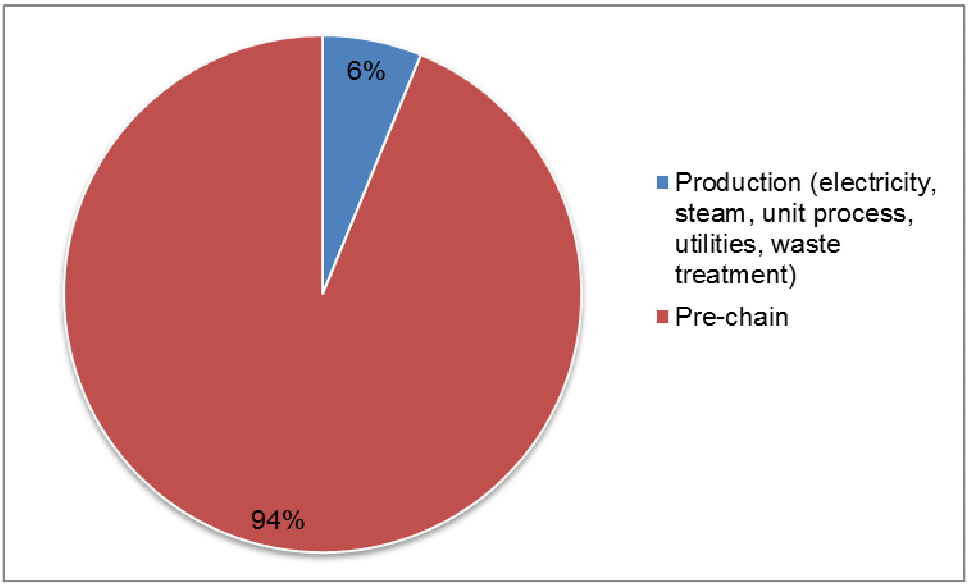


Figure 5: *Contribution to primary energy demand per segment*

Water Use and Consumption

Table 7 shows the water use at cradle-to-gate level. Water use (incl. fresh- and seawater; blue- and green water) equals the measured water input into a product system or process. Water use is determined by total water withdrawal (water abstraction).

Table 7: *Water use (fresh- & seawater; blue- & greenwater) per 1kg aliphatic isocyanate (cradle-to-gate)*

Input	Value [kg]
Water (ground water)	36.3
Water (lake water)	63.3
Water (rain water)	1.2
Water (river water)	3342.2
Water (sea water)	1.5
Water (fossil groundwater)	0.0
Overall water use [kg]	**3444.5**

Table 8 provides the corresponding freshwater part in the water balance. Freshwater is naturally occurring water on the Earth's surface in ponds, lakes, rivers and streams, as ice, and underground as groundwater in aquifers and underground streams. The term specifically excludes seawater and brackish water. Blue water refers to surface and groundwater used.

Table 8: Freshwater (blue water; not including rain water) use and consumption per 1kg aliphatic isocyanate (cradle-to-gate)

Input	**Value [kg]**
Water (ground water)	36.3
Water (lake water)	63.3
Water (river water)	3342.2
Water (fossil groundwater)	0.0
Total fresh water use [kg]	**3441.8**

Output	**Value [kg]**
Water (river water from technosphere, cooling water)	41.7
Water (river water from technosphere, turbined)	3360.0
Water (river water from technosphere, waste water)	11.7
Water (lake water from technosphere, cooling water)	0.0
Water (lake water from technosphere, turbined)	0.0
Water (lake water from technosphere, waste water)	0.0
Total fresh water release from technosphere (degradative use) [kg]	**3413.4**
Total fresh water consumption (blue water)	**28.4**

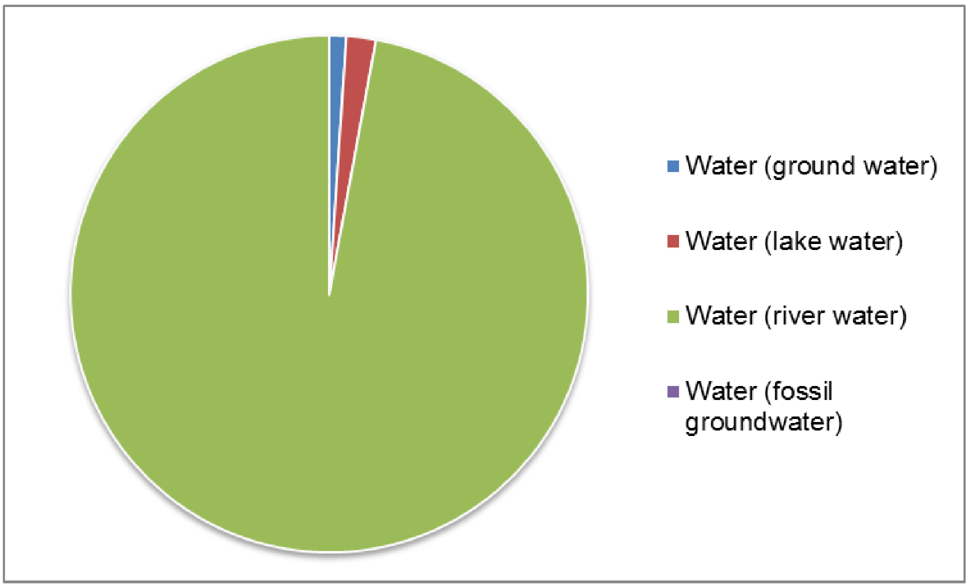


Figure 6: Contribution to freshwater use (blue water not including rain water - Input)

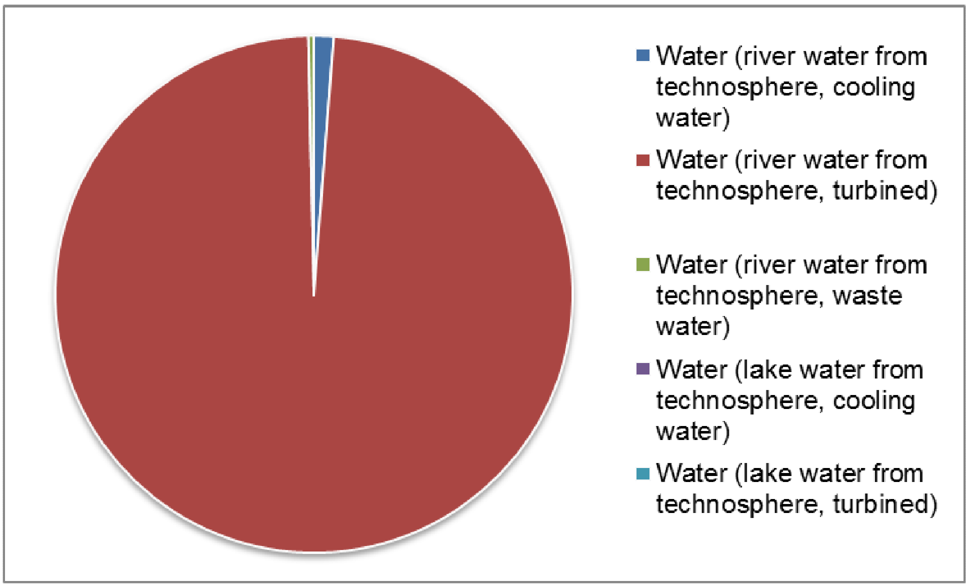


Figure 7: Contribution to water release from technosphere (Output)

Table 9: Water balance table per 1kg aliphatic isocyanate (unit process level)

Input	Value [kg]
Water (cooling water[2])	–
Water (process water)	0.4
Water (deionised)	0.1
Water (ground water)	1.2
Output	**Value [kg]**
Water vapour	0.3
Water (waste water, untreated) to WWTP	0.2
Water direct released to the environment without WWTP	
Water (river water from technosphere, cooling water)	1.0
Water (river water from technosphere, turbined)	0.0
Water (river water from technosphere, waste water)	0.0
Water (sea water from technosphere, cooling water)	0.0
Water (sea water from technosphere, turbined)	0.0
Water (sea water from technosphere, waste water)	0.0
Water (lake water from technosphere, cooling water)	0.0
Water (lake water from technosphere, turbined)	0.0

[2] Cooling water can be processed (softened), deionised, tap, ground, river or sea water, dependent on the location, applied technology and necessary temperature level and site specific frame conditions. Data for differentiation of water amounts used for cooling and processing due to lack of specific meters only partly available.

Air Emission Data

Table 10 shows 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 10: Selected air emissions per 1kg aliphatic isocyanate

Air emissions	kg
Carbon dioxide, fossil (CO_2, fossil)	5.8
Carbon monoxide (CO)	2.8E-03
Sulphur dioxide (SO_2)	4.6E-03
Nitrogen oxides (NO_x)	6.6E-03
Particulate matter ≤ 10 µm (PM 10)	3.2E-04

Wastewater Emissions

Table 11 shows 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 11: Selected water emissions per 1kg aliphatic isocyanate

Water emissions	kg
Biological oxygen demand after 5 days (BOD 5)	6.7E-05
Chemical oxygen demand (COD)	7.0E-04
Total organic carbon (TOC)	2.6E-05

Solid Waste

Table 12: Solid waste generation per 1kg aliphatic isocyanate (key foreground process level)

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous	0	0	0	0	0
Hazardous	0	0	0	0	0
Unspecified	1.2E-01	0	0	0	1.2E-01
Total	1.2E-01	0	0	0	1.2E-01

Life Cycle Impact Assessment

Input

Natural Resources

Table 13: Abiotic Depletion Potential per 1kg aliphatic isocyanate

Natural resources	Value
Abiotic Depletion Potential (ADP). elements [kg Sb eq]	9.3E-06
Abiotic Depletion Potential (ADP). fossil fuels [MJ]	124.0

Output

Climate Change

Table 14: Global Warming Potential (100 years) per 1kg aliphatic isocyanate

Climate change	kg CO_2 eq.
Global Warming Potential (GWP)	6.5

Acidification

Table 15: Acidification Potential per 1kg aliphatic isocyanate

Acidification of soils and water bodies	g SO_2 eq.
Acidification Potential (AP)	9.8

Eutrophication

Table 16: Eutrophication Potential per 1kg aliphatic isocyanate

Eutrophication of soils and water bodies	g PO_4^{3-} eq.
Eutrophication Potential (EP), total	1.6

Ozone Depletion

Table 17: Ozone Depletion Potential per 1kg aliphatic isocyanate

	g CFC-11 eq.
Ozone Depletion Potential (ODP)	2.1E-05

Summer Smog

Table 18: Photochemical Ozone Creation Potential per 1kg aliphatic isocyanate

	g Ethene eq.
Photochemical Ozone Creation Potential	2.2

Dust & Particulate Matter

Table 19: PM10 emissions per 1kg aliphatic isocyanate

Particulate matter	g PM10 eq.
Particulate matter ≤ 10 µm. total	3.2E-01
Particulate matter ≤ 10 µm (direct emissions)	0.0
Particulate matter ≤ 10 µm. secondary	3.2E-01

Dominance Analysis

Table 20 shows the main contributions to the results presented above. An average based on the arithmetic mean from the different technologies of the participating producers is used.

Precursors and process displays the results of the supply chain, i.e. the main input materials. These data refer to direct industry data, complemented with background data of the GaBi database 2011 [GaBi 5 2011]. Other chemicals are materials used in small amounts for the last considered unit process. Utilities cover the environmental impact for water conditioning and inert gas.

In all analysed environmental impact categories, intermediates contribute 89% or more of the total impact. The use of high quality data for the LCI of the supply chain is therefore decisive to the environmental profile of aliphatic isocyanate.

Table 20: Dominance analysis of impacts per 1kg aliphatic isocyanate

	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.]
Precursors and process*	93.0%	99.1%	93.4%	88.9%	90.2%	92.0%	98.6%
Other chemicals	0.8%	0.2%	0.8%	0.5%	1.0%	0.6%	0.5%
Utilities**	0.1%	0.2%	0.0%	0.1%	0.1%	0.1%	0.0%
Electricity	2.5%	0.1%	2.1%	4.0%	4.2%	2.5%	1.4%
Thermal Energy	3.5%	0.4%	3.6%	6.4%	4.1%	4.2%	-0.2%
Transport	0.1%	0.0%	0.1%	0.1%	0.4%	0.5%	-0.5%
Process waste treatment	0.0%	0.0%	0.0%	0.0%	0.0%	0.1%	0.0%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

* Precursors and process include diamines, phosgene, urea, PACM, and direct process emissions

** Utilities include e.g. inert gases, compressed air, process water, etc.

The negative values for thermal energy and transport in the impact category POCP result from Nitrogen Monoxide emissions, which are formed in the generation of thermal energy and in transportation processes. Nitrogen monoxide emissions are assigned with a negative characterisation factors. As the amount of Nitrogen monoxide in some cases exceeds the amount of other emissions to air (which contribute with a positive characterization factor) the total value for POCP gets negative.

Review

Review Details

As part of the European Aliphatic Isocyanates Producers Association (ALIPA) programme management and quality assurance, DEKRA Consulting GmbH conducted an external independent critical review of this work. The outcome of the critical review is reproduced below.

The subject of this critical review was the development of an Eco-profile for aliphatic isocyanates. Five different products from two manufacturers were considered. For confidentiality reasons, an unweighted, arithmetic industry average was created, accepting the systemic variance. This approach had been discussed with and agreed by the participating companies. From a reviewer perspective this seems reasonable and the best possible approach under the given circumstances. For future updates, a weighted average dataset is recommended in order to represent the actual volumes sold on the EU market. However, the confidentiality issue needs to be solved first.

The project included milestone meetings with representatives of all participating producers, the LCA practitioner and the reviewer. In addition, a review meeting between the LCA practitioner and the reviewer was held, which included a model and database review, and spot checks of data and calculations. The final Eco-profile report was also reviewed by representatives of the participating organisations and the reviewer. All questions and recommendations were discussed with the LCA practitioner, and the report was adapted and revised accordingly.

The two manufacturers participating to this Eco-profile cover over 80% of the European aliphatic isocyanates production in 2010. Data for the upstream supply chain until the precursors and all relevant background data (such as energy and auxiliary materials) are taken from the GaBi 5 database.

For the average aliphatic isocyanate, the precursors were shown to have the most substantial influence on the results (more than 88%). Calculation and reporting were subject to extensive analysis and review.

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 quality3.

The critical review confirms that this Eco-profile adheres to the rules set forth in the 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).

As a result, this dataset is assessed to be a reliable and good quality representation of aliphatic isocyanates production in Europe.

Compliance with ILCD Entry-level Requirements

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[3] 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.

Table 21: General review reporting items (reproduced with kind permission of JRC)

REVIEW REPORTING			
General information			
Data set name	**Aliphatic Isocyanates**		
Data set UUID and version number	n/a		
Data set locator (e.g. Permanent URI, URL, contact point, or database name and version, etc.)	n/a		
Data set owner	European Aliphatic Isocyanates Producers Association (ALIPA)		
Review commissioner(s)	European Aliphatic Isocyanates Producers Association (ALIPA)		
Reviewer name(s) and affiliation(s), contact	Christina Bocher, DEKRA Consulting GmbH		
Review type applied	Independent external		
Date of review completion (DD/MM/YYYY)	18/12/2014		
Reviewed against / Compliance system name	ILCD Data Network – Entry-level requirements		
Reviewer assessment:			
Aspect	**Yes**	**No**	**Comments**
Quality compliance (ISO 14040 & 14044) fulfilled (see Table 21)	X		
Method compliance (ISO 14040 & 14044) fulfilled and documented in data set	X		
Nomenclature compliance (see Table 222) fulfilled	X		
Documentation compliance (see Table 222) fulfilled	X		
Review compliance (Independent external review report) fulfilled	X		
Compliant with ISO 14040 & 14044	X		
Overall compliant with compliance system	X		
Date, location, reviewer signature	18 December 2014, Stuttgart, Germany		

Table 212: Specific/detailed review reporting items for LCI data set: quality compliance (ISO 14040 & 14044; reproduced with kind permission of JRC)

ITEMs	Comments
Time-related coverage/representativeness: "age of data and the minimum length of time over which data should be collected" "qualitative assessment of the degree to which the data set reflects the true population of interest"	**Very Good** Foreground: 12 month averages representing the year 2010. Background: 2008—2010 Maximum temporal validity until 2020. (p.9)
Geographical coverage/representativeness: "geographical area from which data for unit processes should be collected to satisfy the goal of the study" "qualitative assessment of the degree to which the data set reflects the true population of interest"	**Very good** European production average (data from 5 production sites from 2 companies) Fuel and energy inputs in the system reflect average European conditions and whenever applicable, site-specific conditions were applied, to reflect representative situations. (p.12)
Technology coverage/representativeness: "specific technology or technology mix" "qualitative assessment of the degree to which the data set reflects the true population of interest"	**Fair** Reasonably similar technology mix, representing European production (see above). For each of the five aliphatic isocyanates the typical European technology was applied. The average aliphatic isocyanate declared in this Eco-profile is a technological arithmetic average of the five considered products, with a systematic variation. › 80% of the European production (EU-27) in 2010. (p.11)
Precision: "measure of the variability of the data values for each data expressed (e.g. variance)"	**n/a** Relevant foreground data is primary data, or modelled based on primary information sources of the owners of the technologies. See Uncertainty below for explanation of "n/a" rating. (p. 13)
Completeness: "percentage of flow that is measured or estimated"; assessed on level of process	**Good** Primary data used for the gate-to-gate production covered all related flows in accordance with the cut-off criteria, i.e. at least 95 % of mass and energy of the input and output flows, and 98 % of their environmental relevance (according to expert judgment) were considered. (p.13)
Consistency: "qualitative assessment of whether the study methodology is applied uniformly to the various components of the analysis"	**Very Good** To ensure consistency, only primary data of the same level of detail were used. While building up the model, cross-checks ensured the plausibility of mass and energy flows. The methodological framework is consistent throughout the whole model as the same methodological principles are used both in foreground and background system. (p.13)
Sources of the data: Appropriateness of use primary/secondary data source	The main data source was a primary data collection from European producers, providing site-specific gate-to-gate production data for processes under operational control of the participating companies. Data for the upstream supply chain until the precursors and all relevant background data are taken from the GaBi database. (p.10)
Uncertainty of the information (e.g. data, models and assumptions).	Variation of single data was not recorded. Variation of the model/dataset not applicable due to vertical average of production lines and technologies. Hence, precision

ITEMs	Comments
	above was rated “n/a”. Critical elements within the model include: • Average aliphatic isocyanate based on arithmetic averaging of the five isocyanates (p.10—11)

Table 222: Specific/detailed review reporting items for LCI data set: nomenclature and documentation (reproduced with kind permission of JRC)

ITEMs	Comments
Nomenclature	
Correctness and consistency of applied nomenclature	Yes – database format is aligned and compatible with ILCD requirements (consistent nomenclature).
Documentation	
Appropriateness of documentation extent (see document “Documentation of LCA data sets”)	Yes – meta-data completed and appropriate; documentation aligned with ILCD standards.
Appropriateness of documentation form (ILCD Format)	Yes – Database format is aligned and compatible with ILCD requirements (consistent format of meta-data and content).

Reviewer Name and Institution

Christina Bocher, Consultant, Sustainability & Performance Excellence, DEKRA Consulting GmbH, Stuttgart, Germany

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