Date: 06/06/2017

Environmental Fact Sheet (#15)

Diethanolamine (DEA)

petrochemical precursor

Substance Identification			
IUPAC Name	2,2'-iminodiethanol	**CAS Number**	111-42-2
Other Names	Diethanolamine; N,N-Diethanolamine; Di(2-hydroxyethyl)amine; Iminodiethanol		
Molecular Formula	C4H11NO2	Structural formula : 	

Physical/Chemical Properties [1]	
Molecular Weight	105,14 g/mol
Physical state	Solid (at 20°C and 1013 hPa). Sometimes liquid
Appearance	Colourless. crystals (prisms) or syrupy liquid (above 82 degrees F)
Odour	Ammonia like
Density	1097.4 kg/m^3 (at 20°C)
Melting Points	27°C (at 1013 hPa)
Boiling point	269.9°C (at 1013 hPa). At and above 200 °C, decomposition can clearly be observed
Flash Point	176°C (at 1013 hPa)
Vapour Pressure	0.00008 hPa (at 20°C)
Water Solubility	Totally miscible (954 g/l at 20°C)
Flammability	Must be preheated before ignition will occur, does not react with water
Explosive Properties	No data available
Surface Tension	No data available
Octanol/water Partition coefficient (Kow)	$\log K_{OW} = -2.46$ (at 25°C)
Product and Process Description	Diethanolamine is used as a precursor of diethanolamide (alkanolamides) for the production of the non-ionic cocamide diethanolamine. Diethanolamine (DEA) is one of several ethanolamines (monoethanolamine, diethanolamine, triethanolamine) produced through the highly exothermic reaction of ethylene oxide with liquid ammonia in excess at moderate temperatures and sufficient pressure to prevent vaporization of both reactants. The amount of ethylene oxide is carefully controlled to ensure full reaction. The reaction products, including excess ammonia and water, are separated through fractional distillation and unconsumed ammonia and water are recycled [5]. The reaction mixture consists of 73.1% monoethanolamine, 3.85% of triethanolamine and 23.1% of diethanolamine. This product composition only depends on the molar excess of ammonia. The higher the proportion of ammonia, the more monoethanolamine is formed. Recycling of mono- or diethanolamine as well as a separate treatment with ethylene oxide can shift the product proportion to di- and triethanolamine.
Application	Diethanolamine and derivatives are commonly used as intermediates in the production of detergents, emulsifiers and textile as well as leather chemicals. They are also used in the production of medicinal soaps and rinse-off cosmetics as well as cutting and drilling oils; at room temperature it is a viscous

	liquid.

Life Cycle Assessment

General Introduction

These Environmental Fact Sheets are a product of the *ERASM Surfactant Life Cycle & Ecofootprinting (SLE)* project. The objective of this project was to establish or update the current environmental profile of 15 surfactants and 17 precursors, taking into consideration actual surfactant production technology and consistent high quality background data.

The Fact Sheets are based upon life cycle assessment (LCA) and have been prepared in accordance with the ISO standard [ISO 14040: 2006 and ISO 14044: 2006]. In addition, the project follows the ILCD (2010) handbook. This Fact Sheet describes the cradle-to-gate production for Diethanolamine (DEA). DEA is a surfactant precursor.

The ERASM SLE project recommends to use the data provided in a full 'cradle-to-grave' life cycle context of the surfactant in a real application.

Further information on the ERASM SLE project and the source of these datasets can be found in [2].

The full LCI can be accessed via www.erasm.org or via http://lcdn.thinkstep.com/Node/

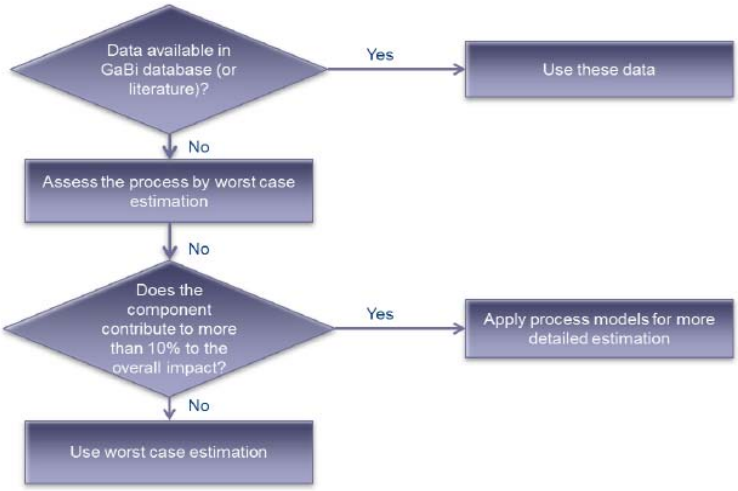
Goal and Scope of ERASM SLE Project [2]

The main goal was to update the existing LCI inventories [3] for the production of Diethanolamine.

Temporal Coverage	Data collected from literature represents DEA production in the year 2011. Background data have reference years from 2008 to 2010 for electricity and thermal energy processes. The dataset is considered to be valid until substantial technological changes in the production chain occur.
Geographical Coverage	LCI covers European conditions. The geographical representativeness for Diethanolamine was considered 'good'.
Technological Coverage	The technological representativeness for Diethanolamine was considered 'good'. Figure 1 provides a schematic overview of the production process of Diethanolamine.
Declared Unit	In ERASM SLE project the declared unit (functional unit) and reference flow is one thousand kilogram (1000 kg) of surfactant active ingredient. This was the reference unit also used in [3]. Functional Unit: 1 metric tonne of Diethanolamine 100% active substance.
Cradle-to Gate System Boundaries	(see table below)
Assumptions and Limitations	The modelling of the dataset is based on secondary data from literature. The catalyst was omitted because of missing relevant information. It was not possible to collect primary industry data. In this case the amounts of electricity and thermal energy as well as cooling water were estimated using different methods: extrapolation, approximation with similar chemicals, molecular structure-based models and process models following the recent production technology to estimate life cycle impacts of chemical compounds (see flowchart below).

Cradle-to Gate System Boundaries:

Included	Excluded
Ammonia production	Construction of major capital equipment (Infrastructure)
Ethylene oxide production (this production is further explained in the Eco Profile fact sheet of the precursor Ethylene oxide (#8))	Maintenance and operation of support equipment
Energy production	Human labor and employee transport
Utilities	Packaging
Transportation processes for the main materials	
Water use and treatment of waste water	
Treatment of wastes	

<table>
<tr><td></td><td colspan="2">
</td></tr>
<tr><td>Cut-off Criteria [4]</td><td colspan="2">No significant cut-offs were used. The LCI study included all material inputs that had a cumulative total (refers to unit process level) of at least 98% of the total mass inputs to the unit process, and included all material inputs that had a cumulative total of at least 98% of total energy inputs to the unit process.
The study included any material that had environmental significance in its extraction, manufacture, use or disposal, is highly toxic, dangerous for the environment, or is classified as hazardous waste.
The sum of the excluded material flows did not exceed 5% of mass, energy or environmental relevance.</td></tr>
<tr><td rowspan="2">Calculation Rules</td><td>Allocation</td><td>Price allocation was applied for Diethanolamine in the foreground system. Allocation to the co-products has been performed based on market value considering allocation by price for 1 kg of the product DEA.</td></tr>
<tr><td>Aggregated data</td><td>From public data and literature research.</td></tr>
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Life Cycle Inventory and Impact Assessment [2]

Based on the LCI data an environmental impact assessment was performed for the indicators Primary Energy Demand (PED) and Global Warming Potential (GWP). Other impacts may be calculated from the full LCI dataset.

Primary Energy Demand (PED): An analysis of the inventory data showed that the PED impact is mainly caused by the use of ethylene oxide, ammonia and process steam. The precursors ethylene oxide and ammonia represent the highest input by mass and contribute 63% and 14% to the total primary energy demand. The applied process steam contributes 19% to PED. The remaining percentages (4%) are caused by electricity supply, nitrogen use, direct emissions, water use, waste and waste water treatment.

Global Warming Potential (GWP): An analysis of the inventory data showed that the GWP impact is mainly caused by the use of ethylene oxide, ammonia and process steam. The precursors ethylene oxide and ammonia represent the highest input by mass and contribute 43% and 26% to the total global warming potential. The applied process steam contributes 28% to GWP. The remaining percentages (3%) are caused by electricity supply, nitrogen use, direct emissions, water use, waste and waste water treatment.

Table 1. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of Diethanolamine 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	905
Primary energy demand from fossil materials (net calorific value)	MJ	51864
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	52769
Air emissions related to Global Warming Potential		
Carbon uptake	kg CO_2 equiv.	-45.2
Carbon dioxide, fossil	kg	1959
Carbon dioxide, biotic	kg	52
Carbon dioxide, from land use, land use change and peat oxidation	kg	-
Methane	kg	6.03
Nitrous oxide (laughing gas)	kg	0.35
NMVOC emissions	kg	1.26
*Total GWP (according to [**IPCC 2007**])*	*t CO_2-equiv.*	*2.22*

References for the ERASM SLE Project

Data Owner and Commissioner of the study	ERASM (Environment & Health Risk Assessment and Management). A research partnership of the Detergents and Surfactants Industries in Europe (www.erasm.org).
LCA Practitioner	thinkstep AG (www.thinkstep.com)
Reviewers	Prof. Walter Kloepffer, LCA Consult Mrs. Charlotte Petiot and Dr. Yannick Leguern, BiolS by Deloitte
References	[1] ECHA. http://echa.europa.eu [2] Schowanek. D *et al*. (2017). New and Updated Life Cycle Inventories for Surfactants used in European Detergents: Summary of the ERASM Surfactant Life Cycle and Ecofootprinting Project. Int J. LCA, in press. [3] CEFIC-Franklin (1994). Resource and environmental profile analysis of petrochemical and oleo chemical surfactants produced in Europe. Phase II Final Report, Franklin Associates, LTD. [4] PLASTICSEUROPE (2011). Eco-profiles and Environmental Declarations – Life Cycle Inventory (LCI) Methodology and Product Category Rules (PCR) for Uncompounded Polymer Resins and Reactive Polymer Precursors, version 2.0. [5] Ullmann's Encyclopedia of Industrial Chemistry (2010), John Wiley & Sons, Inc., Hoboken, USA.

Figure1. Production process of Diethanolamine.