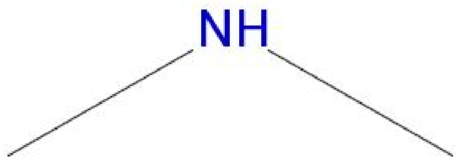
Date: 06/06/2017

Environmental Fact Sheet (#17)
Dimethylamine (DMA)

petrochemical precursor

Substance Identification

IUPAC Name	N-methylmethanamine	**CAS Number**	124-40-3
Other Names			
Molecular Formula	C2H7N	Structural formula: 	

Physical/Chemical Properties [1]

Molecular Weight	45 g/mol
Physical state	Gaseous
Appearance	Colorless
Odour	Fish-, ammonia-like odor
Density	Vapour density: 2.013 kg/m^3 at 0 °C Liquid density: 0.67 kg/l at 0°C
Melting Points	-92.2 °C
Boiling point	7 °C
Flash Point	20 °F (-7°C)
Vapour Pressure	1520 mm Hg (2.026 bar) at 25°C
Water Solubility	Very soluble (> 10000 mg/L)
Flammability	Extremely flammable liquified gas
Explosive Properties	Explosive
Surface Tension	26.34 mN/m at 25 °C
Octanol/water Partition coefficient (Kow)	log K_{OW} =-0.274 at 25°C
Product and Process Description	Dimethylamine belongs to the group of lower alkylamines. Dimethylamine is a surfactant precursor. Methylamines in general are important intermediates for the production of herbicides, pharmaceuticals, detergents, insecticides as well as solvents. In this project, Dimethylamine serves as a precursor to produce the tertiary amine, Lauryldimethylamine. The industrially common production process for lower alkylamines in general is the stepwise methylation of ammonia with the appropriate alcohol over suitable catalyst. 1st step) the dehydrogenation of the alcohol to the carbonyl compound takes place. 2nd step) ammonia is added to obtain the appropriate enamine or imine, which is hydrogenated to the corresponding amine. During the whole process hydrogen is added to prevent side reactions. In case of Dimethylamine the reactants are methanol and ammonia. In this reaction, the product is always a mixture of primary, secondary, and tertiary amines. The primary amine formed initially can react further with one or two molecules of alcohol. The received distribution of the products depends on the amount of ammonia, residence time and temperature. While the initial conversion of the alcohol to the primary amine is close to thermo neutral, the formation of secondary and tertiary amines is exothermic. The reactants are generally used in excess and recycled to the synthesis reactor. The formed water is separated and fed to a waste water treatment system [5] [6].

Application	Precursor with broad applications.

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 Dimethylamine. Dimethylamine is a petrochemical 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/

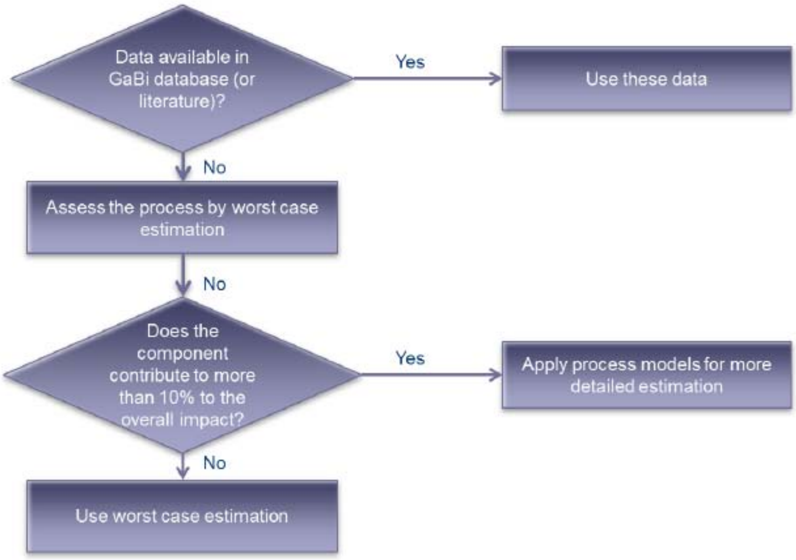
Goal and Scope of ERASM SLE Project [2]

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

Temporal Coverage	Data collected for production refer to literature research covering recent production technology. 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	Data for Dimethylamine came from internal database and covers European conditions. The geographical representativeness for Dimethylamine was considered 'good'.
Technological Coverage	The technological representativeness for Dimethylamine was considered 'good'. Figure 1 provides a schematic overview of the production process of Dimethylamine.
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 Dimethylamine 100% active substance.
Cradle-to Gate System Boundaries	(see table below)
Assumptions and Limitations	This model was based on secondary data from literature. Therefore the modeled data are according to stoichiometric amounts with respect to the yield of the reaction. The catalyst and the amount of hydrogen needed for the catalyst were neglected due to missing valuable information and the amounts of process 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 (cf. flowchart below).

Cradle-to Gate System Boundaries:

Included	Excluded
Ammonia production	Construction of major capital equipment (Infrastructure)
Methanol production	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>Allocation between the co-products was carried out by mass per one kilogram of product DMA (amounts of the reactants were calculated by stoichiometric rules). The reaction mixture consists of 23% monomethyl amine, 43.7% of trimethyl amine and 33.3% of dimethyl amine.</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 shows that the PED impact was mainly caused by the raw materials ammonia and methanol and the production of process steam. T he precursors, ammonia and methanol, represent the highest input by mass and contribute 18% and 59% to the total primary energy demand. Further, applied process steam contributed 23% to PED. The remaining contribution was due to electricity supply, direct emissions, water use, waste and waste water treatment as well as the treatment of waste, account together for 1% of the total primary energy demand.

Global Warming Potential (GWP): An analysis of the inventory data showss that the GWP impact was mainly caused by the raw materials ammonia and methanol and the production of process steam. The precursors, ammonia and methanol, represent the highest input by mass and contribute 34% and 28% to the total global warming potential. Further, applied process steam contributed 36% to GWP. The remaining contribution was due to electricity supply, direct emissions, water use, waste and waste water treatment as well as the treatment of waste, account together for 1% of the total primary energy demand.

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

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	642
Primary energy demand from fossil materials (net calorific value)	MJ	78578
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	79220
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-23.1
Carbon dioxide, fossil	kg	2706
Carbon dioxide, biotic	kg	36
Carbon dioxide, from land use, land use change and peat oxidation	kg	-
Methane	kg	6.59
Nitrous oxide (laughing gas)	kg	0.61
NMVOC emissions	kg	1.04
*Total GWP (according to [***IPCC 2007***])*	*t CO_2-equiv.*	*3.07*

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] Arpe, H.-J. (2010). Industrial Organic Chemistry, 5th Edition, Wiley-VCH Verlag. [6] Ullmann's Encyclopedia of Industrial Chemistry (2010). John Wiley & Sons, Inc., Hoboken, USA.

Figure 1. Production process of Dimethylamine.