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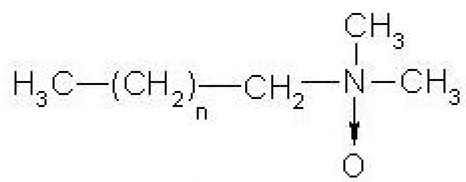
Environmental Fact Sheet (#20)

C12-14 Amine Oxide (Lauryldimethylamine oxide – C12-14 AO)

oleochemical non-ionic surfactant

Substance Identification			
IUPAC Name	Amines, C12-14 (even numbered)-alkyldimethyl, N-oxides	**CAS Number**	308062-28-4
Other Names	Lauryldimethylamine oxide		
Molecular Formula	UVCB substance (substances of Unknown or Variable composition, Complex reaction products or Biological materials), no univocal molecular formula available	Structural formula:  n = 10 or 12	

Physical/Chemical Properties [1]	
Molecular Weight	229.4-257.5 g/mol
Physical state	Solid
Appearance	White powder
Density	716 kg/m^3 at 23 °C
Melting Points	126-136 °C
Boiling point	Study scientifically unjustified
Flash Point	Study technically not feasible
Vapour Pressure	$1.7*10^{-06}$ and $7.5*10^{-05}$ Pa at 25°C
Water Solubility	409.5 g/L
Flammability	Non flammable
Explosive Properties	Study scientifically unjustified
Surface Tension	34.1 mN/m at 20 °C
Octanol/water Partition coefficient (Kow)	log K_{OW} =1.85-2.69
Product and Process Description	Lauryldimethylamine oxide in a neutral aqueous solution is regarded as a non-ionic surfactant. Amine oxides are produced by the reaction of tertiary amines such as Alkyldimethylamine with hydrogen peroxide in a two-phase system containing a large volume of water yielding dilute products typically containing <35% active [5]. The reaction is a continuous process. In the primary step the tertiary amine, a hydrogen peroxide solution, deionized water as well as the catalyst and its chelate are pumped continuously at controlled rates into a stirred reactor. This oxidation reaction is exothermic and yields approximately 95% of the desired product. To generate more product, the outflow of the first reactor is passed to a second reactor, which extends the yield of the amine oxide to approximately 99%. The received product outflow is cooled to maintain color.
Application	Widely used as constituents of dishwasher detergents, shampoos, and soaps.

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 C12-14 Amine Oxide (AO). AO is an oleochemical surfactant.
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 Amine Oxide and its main precursors/intermediates.

Temporal Coverage	Data collected represents a 12 month averages of AO production in the year 2011, to compensate seasonal influence of data. Background data have reference years from 2008 to 2010. The dataset is considered to be valid until substantial technological changes in the production chain occur.
Geographical Coverage	Primary production data for Amine Oxide production were from different suppliers in Europe. The geographical representativeness for C12-14 AO was considered 'very good'.
Technological Coverage	The technological representativeness for C12-14 AO was considered 'good'. Figure 1 provides a schematic overview of the production process of C12-14 Amine oxide.
Representativeness for market volume	>70% (Represented market volume (in mass) covered by primary data used in ERASM SLE project).
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 C12-14 AO 100% active substance.
Cradle-to Gate System Boundaries	see table below
Assumptions and Limitations	Transportation was only considered for the main materials (covers about 90% of the mass of all inputs), other transportation was not considered. Some important transports were estimated by European standard distances due to lack of specific information.

Cradle-to Gate System Boundaries:

Included	Excluded
Alkyldimethylamine production (this production is further explained in the Eco Profile fact sheet of the precursor C12-14 Dimethylamine (Tertiary Amine) (#19))	Construction of major capital equipment (Infrastructure)
Hydrogen peroxide production (this production is further explained in the Eco Profile fact sheet of the precursor Hydrogen peroxide (#18))	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	

Cut-off Criteria	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.	
Calculation Rules	Allocation	For C12-14 Amine Oxide production, allocation was not applied to the foreground system. However, allocation was applied for some background data (mass allocation for the renewable precursors PKO and CNO).
	Aggregated data	Vertical averaging was considered (as long as the final product was the same, different processes with common product intermediates can be aggregated in the average).

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.

Table 1. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of C12-14 Amine Oxide 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	37435
Primary energy demand from fossil materials (net calorific value)	MJ	39038
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	76473
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	- 4173.48
Carbon dioxide, fossil	kg	1638.5
Carbon dioxide, biotic	kg	1736.4
Carbon dioxide, from land use and land use change	kg	2653.9
Methane	kg	24.9
Nitrous oxide (laughing gas)	kg	0.899
NMVOC emissions	kg	2.43
*Total GWP (according to [**IPCC 2007**])*	*t CO_2-equiv.*	*2.75*

Primary Energy Demand (PED): Contributions to the PED come about equally from the renewable and fossil precursors.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP impact is mainly caused by the production of the C12-14 dimethylamine (more than 85% of total) which is also the highest input by mass. Furthermore hydrogen peroxide is also a high input by mass and contributes with 10 - 15% to the total GWP. Electricity and thermal energy generation as well as utilities, process waste treatment account for less than 2% of the total value of GWP.

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, BioIS by Deloitte Dr. Yannick Schmidt (2.0 LCA consultant)
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] Zoller et al. (2009). Handbook of Detergents: Part F: Production, Volume 142, CRC Press.

Figure 1. Production process of C12-14 Amine Oxide.