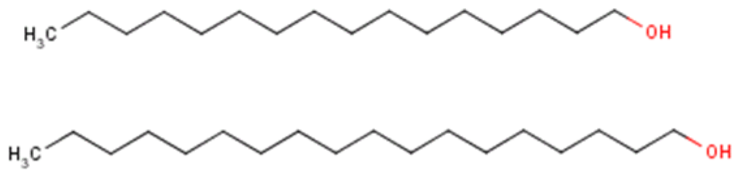
Date: 06/09/2017

Environmental Fact Sheet (#13)

C16-18 Fatty Alcohol

oleochemical precursor

Substance Identification			
IUPAC Name	Alcohols, C16-18	**CAS Number**	67762-27-0
Other Names	Cetearyl Alcohol		
Molecular Formula	C16H34O / C18H380	Structural formula (example): 	

Physical/Chemical Properties	
Molecular Weight	242.44 - 270.49 g/mol
Physical state	Liquid
Appearance	No data available
Odour	No data available
Density	No data available
Melting Points	No data available
Boiling point	No data available
Flash Point	No data available
Vapour Pressure	No data available
Water Solubility	No data available
Flammability	No data available
Explosive Properties	No data available
Surface Tension	No data available
Octanol/water Partition coefficient (Kow)	No data available
Product and Process Description	C16-18 fatty alcohol is a surfactant precursor. C16-18 fatty alcohol (oleo) is produced from natural sources which contain fatty acids in the form of triglycerides that can be hydrogenated after suitable pre-treatment. For the production of C16–18 alcohols, preferably palm oil, and tallow are used. The production stages of C16-18 fatty alcohol are [4]: 1) Contaminants such as phosphatides, sterols, or oxidation products and impurities such as seed particles, dirt, and water are removed in a cleaning stage, which includes refining by treatment with phosphoric acid, centrifugation, and adsorption, e.g., on charcoal or bentonite. 2) Hydrolyzing of the refined triglycerides to yield fatty acids or trans-esterified with lower alcohols to yield fatty acid esters. 3) The Refined fatty acid methyl esters are used for hydrogenation to generate fatty alcohol.
Application	Fatty alcohols possess good foaming properties and ready biodegradability, and are extensively used as base surfactants for laundry detergent products, shampoo, dishwashing liquids and cleaners. Moreover, C16-18 fatty alcohol finds application as a defoamer, as a solubility retarder for syndets bars, and a consistency giving factor in creams and polishes.

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 C16-18 fatty alcohol. C16-18 is an oleochemical 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 [1].

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

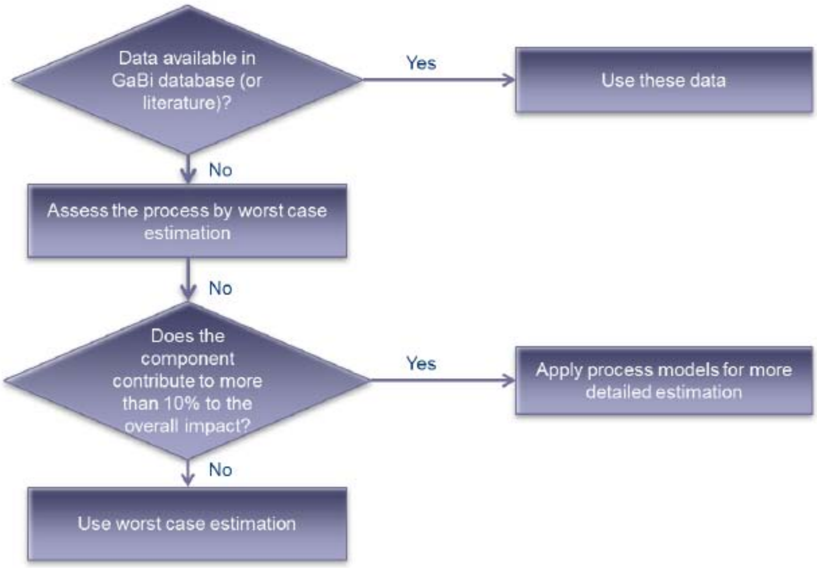
Goal and Scope of ERASM SLE Project [1]

The main goal was to update the existing LCI inventories [2] for the production of C16-18 fatty alcohol.

Temporal Coverage	Data collected for production refer to literature research covering recent production technology. The reference year was set to 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	No primary data collection takes place in this case. Data from literature and expert judgement is used for modelling the European average. The geographical representativeness for C16-18 was considered ' good'.
Technological Coverage	The technological representativeness for C16-18 was considered 'fair'. Figure 1 provides a schematic overview of the production process of C16-18.
Representativeness for market volume	>70% (Represented market volume (in mass) covered by primary data used in ERASM SLE project).
Declared Unit	In the 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 [2]. Functional Unit: 1 metric tonne of C16-18 100% active substance
Cradle-to Gate System Boundaries	see table below
Assumptions and Limitations	The modelled data for fatty alcohol production is based on secondary data from literature [4]. The amounts of energy and cooling water were estimated using different methods: extrapolation, approximation with similar chemicals, molecular structure-based models and process models following the recent production technology (see flowchart below).

Cradle-to Gate System Boundaries:

Included	Excluded
Fatty acid methyl ester production (based on tallow and palm oil)	Construction of major capital equipment (Infrastructure)
Hydrogen 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	



Cut-off Criteria [4]	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 C16-18 production, Allocation methods used for the renewable precursors PO and CNO (allocation mass).
	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 [1]

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. This impact assessment was performed for C16-18 fatty alcohol (tallow) and C16-18 fatty alcohol (palm oil).

C16-18 fatty alcohol (tallow):

Primary Energy Demand (PED): An analysis of the inventory data showed that the main contribution comes from the production of the fatty acid ester (around 79% contribution). Around 13% of the PED is due to the production of hydrogen. The generation of thermal energy contributes with around 5% to PED. The remaining percentages (3%) are caused by electricity generation, cooling water production and the treatment of waste.

Global Warming Potential (GWP): An analysis of the inventory data showed that the main contribution comes from the production of the fatty acid ester (around 80% contribution). This precursor from renewable material is also the highest input related to mass. Around 12% of the GWP are due to the production of hydrogen. The generation of thermal energy contributes with around 4% to GWP. The remaining percentages (4%) are caused by electricity generation, cooling water production and the treatment of waste.

Table 1. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of C16-18 fatty alcohol (tallow) 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	10545
Primary energy demand from fossil materials (net calorific value)	MJ	19719
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	30265
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	- 3945
Carbon dioxide, fossil	kg	1128
Carbon dioxide, biotic	kg	62
Carbon dioxide, from land use, land use change and peat oxidation	kg	0
Methane	kg	51.8
Nitrous oxide (laughing gas)	kg	0.88
NMVOC emissions	kg	2.9
Total GWP (according to [IPCC 2007])	*t CO_2-eq.*	*-1.20*

C16-18 fatty alcohol (Palm oil):

Primary Energy Demand (PED): An analysis of the inventory data showed that the main contribution comes from the production of the fatty acid ester (around 92% contribution). The production of hydrogen causes roughly 5% of the PED. The remaining percentages (3%) are caused by thermal energy, electricity, cooling water and the treatment of waste water.

Global Warming Potential (GWP): An analysis of the inventory data showed that the main contribution comes from the production of the fatty acid ester (around 92% contribution), which is also the main input by mass. The production of hydrogen causes roughly 5% of the GWP. The remaining percentages (3%) are caused by thermal energy, electricity, cooling water and the treatment of waste water.

Table 2. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of C16-18 fatty alcohol (palm oil) 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	50469
Primary energy demand from fossil materials (net calorific value)	MJ	9540
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	60009
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-5361
Carbon dioxide, fossil	kg	537
Carbon dioxide, biotic	kg	2398
Carbon dioxide, from land use, land use change and peat oxidation	kg	4358
Methane	kg	36.2
Nitrous oxide (laughing gas)	kg	1.04
NMVOC emissions	kg	2.89
*Total GWP (according to [***IPCC 2007***])*	*t CO_2-equiv.*	*3.15*

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] 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. [2] CEFIC-Franklin (1994). Resource and environmental profile analysis of petrochemical and oleo chemical surfactants produced in Europe. Phase II Final Report, Franklin Associates, LTD. [3]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. [4] Ullmann's Encyclopedia of Industrial Chemistry (2010). John Wiley & Sons, Inc., Hoboken, USA.

Figure1. Production process of C16-18 Fatty Alcohol.