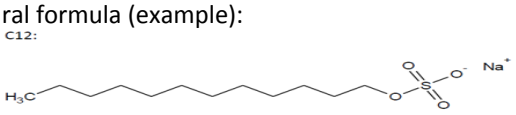
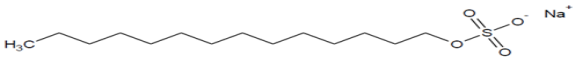
Date: 02/06/2017

Environmental Fact Sheet (#5)

C12-14 and C12-15 Sodium Alkyl Sulphate (C12-14 mix AS)

oleo/petrochemical anionic surfactant

Substance Identification			
IUPAC Name	Sulfuric acid, C12-14-alkyl (even numbered) esters, sodium salts Sulfuric acid, mono C12-15-alkyl esters, sodium salts	**CAS Number**	85586-07-8 (C12-14 AS) 68890-70-0 (C12-15 AS)
Other Names	Sodium Lauryl Sulfate; Sodium Monolauryl sulphate Sodium dodecanesulafte; Sodium Coco Sulfate; dodecyl alcohol; hydrogen sulphate; sodium salt, n-Dodecyl sulphate sodium; Sulfuric acid monodecyl ester sodium salt.		
Molecular Formula	UVCB substance (substances of Unknown or Variable composition, Complex reaction products or Biological materials), no univocal molecular formula available	Structural formula (example): C12:  C14: 	

Physical/Chemical Properties (example for C12-14 AS) [1]	
Molecular Weight	288 - 316 g/mol
Physical state	Solid (at 20°C and 1013 hPa)
Appearance	Colorless or yellow solid
Odour	Odourless
Density	1.155 at 20 °C
Melting Points	Glass transition state at 5 °C and 102 °C
Boiling point	Ca. 187 °C at 1010 mbar
Flash Point	206.5 °C at 1013 mbar
Vapour Pressure	≤0.18 Pa at 20 °C (read-across based on grouping of substances (category approach)) ≤0.97 Pa at 20 °C (estimated by calculation)
Water Solubility	>400 g/l at 20 °C
Flammability	Solid material: not highly flammable Fine powder: flammable
Explosive Properties	Non explosive
Surface Tension	29.9 mN/m at 23 °C
Octanol/water Partition coefficient (Kow)	log K_{OW} = 0.78 at 22 °C
Product and Process Description	Sodium alkyl sulphates are among the oldest oleochemical surfactants produced already since 1930 and are widely used. The chainlength of the alcohol determines the application area. Two main types of AS are covered by the ERASM SLE project, one with a chainlength of C16-18 derived mainly

	from tallow and palm oil, and another type represented here with a chainlength of C12-14 or C12-15. C12-14 AS is an anionic surfactant which can be made from coconut and palm kernel oil (referred to a 'oleo'). The C12-15 AS is the petroleum-based version (referred to as 'petro'). The use of these oils varies between manufacturing sites and fluctuates based on market availability and price. **The inventory described here represents a market mix of the oleo and petro form, as reported to the consultant. C12-14 AS and C12-C15 AS inventories are not reported separately in the SLE study.** C12-14 AS is produced from fatty acids or fatty acid methyl esters through an intermediate product (its precursor: C12-14 fatty alcohol) by hydrogenation. The production stages of C12-14 AS are: Step 1) Refining of triglycerides by treatment with phosphoric acid, centrifugation, and adsorption. Step 2) Hydrolysis of refined triglycerides to yield fatty acids, or transesterified (with methanol) to yield fatty acid methyl esters. Step 3) Hydrogenation of fatty acid methyl esters to generate fatty alcohol. Step 4) Sulphation of C12-14 fatty with sulphur trioxide diluted with inert gas. Step 5) The reaction product leaving the reactor is degassed and neutralised as quickly as possible using sodium hydroxide. Steps 1, 2 and 3 are further explained in the Fact Sheet of the surfactant precursor C12-14 Fatty Alcohol (#3) C12-15 alcohol is an essentially linear surfactant precursor of petrochemical origin. C12-15 alcohol represented in this project is produced from petrochemical feedstock and based on the oxo process. The oxo process (hydroformylation) consists of the reaction of olefins with an H2/CO gas (oxo gas) mixture in the presence of suitable catalysts. The process involves the following steps: oxo reaction, catalyst separation and regeneration, aldehyde hydrogenation and alcohol distillation (see Fact Sheet #4).
Application	Alkyl Sulphates are common components in washing and clearing products.

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 a representative mixture of C12-14 AS (from palm or coconut origin) and C12-15AS (from petrochemical origin) as marketed in Europe.
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 [3,5] for the production of C12-14 mix AS and its main precursors/intermediates.

Temporal Coverage	Data were collected as 12 month averages representing the year 2011. 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.

<table>
<tr><td>Geographical Coverage</td><td>Current data were based on three suppliers from Asia and Europe representing the imported and produced C12-14 mix AS in Europe.
The geographical representativeness for C12-14 AS was considered ‘good’.</td></tr>
<tr><td>Technological Coverage</td><td>The technological representativeness for C12-14 AS was considered ‘good’.
Figure 1 provides a schematic overview of the production process of C12-14 AS.</td></tr>
<tr><td>Representativeness for market volume</td><td>>50% (Represented market volume (in mass) covered by primary data used in ERASM SLE project).</td></tr>
<tr><td>Declared Unit</td><td>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 mix AS 100% active substance.</td></tr>
<tr><td>Cradle-to Gate System Boundaries</td><td>
<table>
<tr><th>Included</th><th>Excluded</th></tr>
<tr><td>C12-14 (oleo) and C12-15 (petro) alcohol production (these productions are further explained in the Eco Profile fact sheet of the precursor C12-14 fatty alcohol (#3) and C12-15 fatty alcohol (#4))</td><td>Construction of major capital equipment (Infrastructure)</td></tr>
<tr><td>Sulphur trioxide production</td><td>Maintenance and operation of support equipment</td></tr>
<tr><td>Sodium hydroxide production</td><td>Human labor and employee transport</td></tr>
<tr><td>Energy production</td><td>Packaging</td></tr>
<tr><td>Utilities</td><td></td></tr>
<tr><td>Transportation processes for the main materials</td><td></td></tr>
<tr><td>Water use and treatment of waste water</td><td></td></tr>
<tr><td>Treatment of wastes</td><td></td></tr>
</table>
</td></tr>
<tr><td>Assumptions and Limitations</td><td>Transportation was considered for the main materials only (i.e. covers about 90% of the mass of all inputs), other transportation was not considered.</td></tr>
<tr><td>Cut-off Criteria [4]</td><td>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>For C12-14 mix AS 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).</td></tr>
<tr><td>Aggregated data</td><td>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).</td></tr>
</table>

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 production of the fatty alcohol contributes 50–60% to the total PED and sodium hydroxide around 10%. Electricity and generation of thermal energy contribute around 20%

to the PED. The remaining contribution is due to consumed utilities, the waste treatment and transport.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP of this production process is mainly caused (with more than 50% contribution) by the fatty alcohol, which is also the highest input by mass. Sodium hydroxide is responsible for approx. 10% of the GWP. Electricity and generation of thermal energy contribute around 20% to the GWP. The remaining contribution is due to consumed utilities, the waste treatment and transport.
The carbon uptake results mainly from the precursor C12-C14 fatty alcohol.

Table 1. Primary Energy Demand and air emissions related to Global Warming per 1 tonne of C12-14 AS/C12-15 AS mix 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	24601
Primary energy demand from fossil materials (net calorific value)	MJ	42154
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	66755
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-2938
Carbon dioxide, fossil	kg	2159
Carbon dioxide, biotic	kg	1053
Carbon dioxide, from land use, land use change and peat oxidation	kg	918
Methane	kg	12
Nitrous oxide (laughing gas)	kg	0.51
NMVOC emissions	kg	1.85
Total GWP (according to [IPCC 2007])	*t CO_2-equiv.*	*1.63*

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	
Reviewers	Prof. Walter Kloepffer, LCA Consult Mrs. Charlotte Petiot and Dr. Yannick Leguern, BiolS by Deloitte Dr. Yannick Schmidt (2.0 LCA Consultants).
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] Stalmans, M. *et al*. (1995). European Life-Cycle Inventory for Detergent Surfactants Production, Tenside Surf. Det. 32 (2), 84-109.

Figure 1. Production process of C12-14 mix AS.