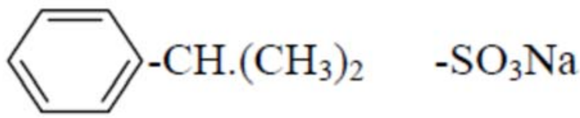
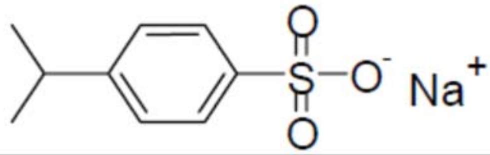
ERASM

Date: 07/06/2017

Environmental Fact Sheet (#30)

Sodium Cumene Sulphonate (SCS)

petrochemical anionic surfactant/hydrotope

<table>
<tr><th colspan="4">Substance Identification</th></tr>
<tr><td>IUPAC Name</td><td>Sodium Cumene Sulphonate</td><td>CAS Number</td><td>28348-53-0</td></tr>
<tr><td>Other Names</td><td colspan="3">Benzenesulfonic acid, (1-methylethyl)-, sodium salt</td></tr>
<tr><td>Molecular Formula</td><td>C9H11NaO3S</td><td colspan="2">Structural formula (without isomer orientation):

Para isomer structure:
</td></tr>
</table>

Physical/Chemical Properties [1]	
Molecular Weight	222.24 g/mol
Physical state	No data available
Appearance	No data available
Odour	No data available
Density	No data available
Melting Points	182 °C
Boiling point	No data available
Flash Point	No data available
Vapour Pressure	1.09×10^{-9} Pa at 25°C
Water Solubility	330 g/l
Flammability	No data available
Explosive Properties	No data available
Surface Tension	35 mN/m at 25 °C
Octanol/water Partition coefficient (Kow)	log K_{OW} = -1,5
Product and Process Description	Sodium cumene sulphonate (SCS) is an anionic surfactant and acts as hydrotropes to modify solubilities, viscosities, and other properties of surfactants and surfactant formulations. SCS is produced by the sulphonation of cumene followed by neutralization with sodium hydroxide. Sulphonation step: involves the use of oleum, a solution of SO3 in sulphuric acid. Neutralization step: The generated aromatic sulphonic acid is converted to their respective salts by neutralization with sodium hydroxide to produce the sodium sulphonate. The neutralization is conveniently done in water, since the sulphonates, and even more so the short alkyl chain hydrotropes, are generally water soluble to the extent of 30–50%. Post-processing step: can involve a solvent extraction to remove sulphones and chemical bleaching. If solvent extraction is done, traces of solvent must be removed by distillation, usually as the

	azeotrope. For a low sulphate product treatment with lime may be necessary.
Application	Hydrotropes are used in a variety of household detergent and cleaning products including laundry powders and liquids, liquid fabric conditioners, liquid and powder laundry bleach additives, hand dishwashing liquid, machine dishwashing liquid, liquid and gel toilet cleaners, and liquid, powder, gel and spray surface cleaners.

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 Sodium Cumene Sulphonate (SCS). SCS is a petrochemical 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 Sodium Cumene Sulphonate and its main precursors/intermediates.

Temporal Coverage	Data collected represents a 12 month averages of SCS 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	Current data are based on three suppliers representing SCS production in Europe. The geographical representativeness for Sodium cumene sulphonate was considered 'very good'.
Technological Coverage	The technological representativeness for Sodium cumene sulphonate was considered 'very good'. Figure 1 provides a schematic overview of the production process of Sodium cumene sulphonate.
Representativeness for market volume	>80% (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 SCS 100% active substance.
Cradle-to Gate System Boundaries	(see table below)

Cradle-to Gate System Boundaries

Included	Excluded
Cumene production (this production is further explained in the Eco Profile fact sheet of the precursor Cumene (#29))	Construction of major capital equipment (Infrastructure)
Sodium hydroxide production	Maintenance and operation of support equipment
Sulphuric acid production	Human labor and employee transport
Energy production	Packaging
Utilities	
Transportation processes for the main materials	
Water use and treatment of waste water	
Treatment of wastes	

<table>
<tr><td>Assumptions and Limitations</td><td colspan="2">Transportation was only considered for the main materials (covers about 90% of the mass of all inputs), other transportation was not considered.</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>For Sodium Cumene Sulphonate production, allocation was not applied to the foreground system. However, allocation was applied for some background data.</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.

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

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	988
Primary energy demand from fossil materials (net calorific value)	MJ	51400
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	52400
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-57.3
Carbon dioxide, fossil	kg	1593
Carbon dioxide, biotic	kg	62
Carbon dioxide, from land use, land use change and peat oxidation	kg	-
Methane	kg	5.05
Nitrous oxide (laughing gas)	kg	0.047
NMVOC emissions	kg	0.92
*Total GWP (according to [***IPCC 2007***])*	*t CO_2-equiv.*	*1.74*

Primary Energy Demand (PED): An analysis of the inventory data shows that the PED impact is mainly caused by the production of the raw materials cumene and sodium hydroxide and generation of thermal energy. The intermediates cumene and sodium hydroxide together contribute 80% to the PED and the thermal energy contributes 6%. The remaining contributions are due to sulphuric acid, electricity, utilities, waste treatment and transport.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP impact is mainly caused by the production of the raw materials cumene and sodium hydroxide and generation of thermal energy. The intermediates cumene and sodium hydroxide together contribute 70% to the GWP and the thermal energy contributes 16%. The remaining contributions are due to sulphuric acid, electricity, utilities, waste treatment and transport.

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] Human & Environmental Risk Assessment on ingredients of household cleaning products – Hydrotropes (Edition 1.0, September 2005). www.heraproject.com [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.

Figure 1. Production process of Sodium Cumene Sulphonate.