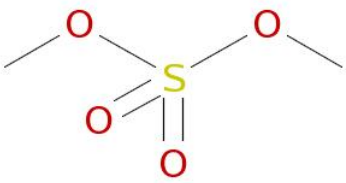
Date: 07/06/2017

Environmental Fact Sheet (#23)
Dimethylsulphate (DMS)

petrochemical precursor

Substance Identification			
IUPAC Name	Dimethyl sulfate	**CAS Number**	77-78-1
Other Names	Sulfuric acid dimethyl ester, DMS		
Molecular Formula	C2H6O4S	Structural formula: 	

Physical/Chemical Properties [1]	
Molecular Weight	126.13 g/mol
Physical state	Liquid
Appearance	Viscous and colourless
Odour	Characteristic of sulfur-containing compounds
Density	1.33 g/cm^3 at 20°C
Melting Points	-31.7 °C at 1013.3 mBar
Boiling point	188 °C at 1013.3 mBar
Flash Point	83 °C
Vapour Pressure	90.3 Pa at 25 °C
Water Solubility	Very soluble (> 10000 mg/L)
Flammability	No data available
Explosive Properties	Non explosive
Surface Tension	40.12 mN/m at 18°C
Octanol/water Partition coefficient (Kow)	log K_{OW} =0.16 (QSAR- estimated value)
Product and Process Description	Dimethyl sulphate (DMS) is one of the commercially most important dialkyl sulphates. DMS is besides triethanolamine and fatty acids a surfactant precursor to produce the cationic surfactants TEA-Quats. The intermediate dimethyl sulphate is industrially produced by the reaction of gaseous dimethyl ether and liquid sulphur trioxide in stoichiometric quantities. The reaction is a continuous process and carried out in water-cooled, vertical aluminium or stainless steel tubes. The removal of dimethyl ether in the technical grade dimethyl sulphate by vacuum distillation over anhydrous sodium sulphate was considered in the model [5].
Application	Dimethyl sulfate is used as a methylating agent in the manufacture of many organic chemicals (surfactants, fabric softeners, pesticides…) It is also used in the manufacture of dyes and perfumes, for the separation of mineral oils, and for the analysis of auto fluids.

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 dimethylsulphate (DMS). DMS 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 Dimethylsulphate.

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	Data for Dimethylsulphate came from the GaBi database and covers European conditions. The geographical representativeness for Dimethylsulphate was considered 'good'.
Technological Coverage	The technological representativeness for Dimethylsulphate was considered 'good'. Figure 1 provides a schematic overview of the production process of Dimethylsulphate.
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 Dimethylsulphate 100% active substance.
Cradle-to Gate System Boundaries	See table below
Assumptions and Limitations	The modelling was conducted based on stoichiometric amounts as indicated in literature with respect to the yield of production. Process energy as well as the amount of cooling water was estimated by similar production processes.
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.

Included	Excluded
Dimethyl ether production	Construction of major capital equipment (Infrastructure)
Sulphur trioxide 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	

	The sum of the excluded material flows did not exceed 5% of mass, energy or environmental relevance.	
Calculation Rules	Allocation	No allocation was applied (the process was modeled for stoichiometric amounts to produce one kilogram of the desired product DMS).
	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 dimethyl sulphate 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	336
Primary energy demand from fossil materials (net calorific value)	MJ	29834
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	30169
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-13.8
Carbon dioxide, fossil	kg	1094
Carbon dioxide, biotic	kg	26
Carbon dioxide, from land use, land use change and peat oxidation	kg	-
Methane	kg	2.97
Nitrous oxide (laughing gas)	kg	0.01
NMVOC emissions	kg	0.48
Total GWP (according to [IPCC 2007])	*t CO_2-equiv.*	*1.18*

Primary Energy Demand (PED): An analysis of the inventory data shows that the PED impact is mainly caused by sulphur trioxide, dimethyl ether and the generation of thermal energy. The reactants sulphur trioxide and dimethyl ether represent the highest input by mass and contribute 30% and 48% to the total primary energy demand. Also the generated thermal energy contributes 20% to PED. In contrast, the reactant sodium sulphate only accounts for 3% to the PED. The remaining percentages are caused by electricity supply, direct emissions, water use, waste water as well as waste treatment.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP impact is mainly caused by sulphur trioxide, dimethyl ether and the generation of thermal energy. The reactants sulphur trioxide and dimethyl ether represent the highest input by mass and contribute 39% and 26% to the total impact of global warming potential. Also the generated thermal energy contributes 29% to GWP. In contrast, the reactant sodium sulphate only accounts for 4% to the GWP. The remaining percentages are caused by electricity supply, direct emissions, water use, waste water as well as waste treatment.

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] Ullmann's Encyclopedia of Industrial Chemistry (2010). John Wiley & Sons, Inc., Hoboken, USA.

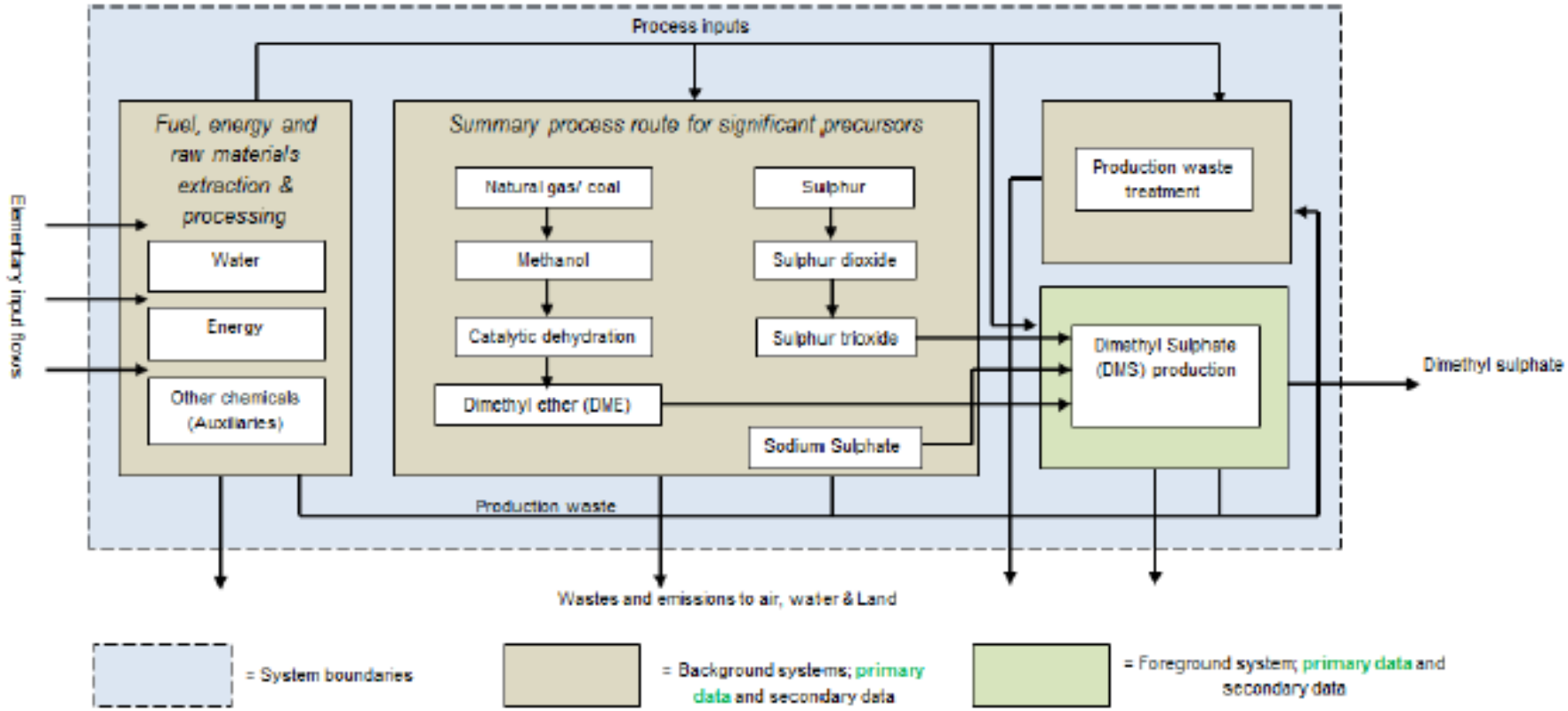



Figure 1. Production process of Dimethyl Sulphate.