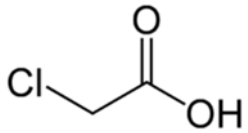
Date: 07/06/2017

Environmental Fact Sheet (#27)

Chloroacetic Acid

petrochemical surfactant precursor

Substance Identification			
IUPAC Name	2-Chloro-ethanoic acid	**CAS Number**	79-11-8
Other Names	3-aminopropyldimethylamine		
Molecular Formula	C2H3ClO2	Structural formula: 	

Physical/Chemical Properties [1]	
Molecular Weight	94.5 g/mol
Physical state	Solid (flakes)
Appearance	White
Odour	No data available
Density	1.64 g/cm³ at 20°C
Melting Points	63°C at 101.325 kPa
Boiling point	190°C at 101.325 kPa
Flash Point	126°C
Vapour Pressure	6 hPa at 20 °C
Water Solubility	Miscible
Flammability	Not highly flammable in contact with water or damp air
Explosive Properties	Non explosive
Surface Tension	73.1 mN/m at 20°C (not surface active)
Octanol/water Partition coefficient (Kow)	log K_{OW} =0.49
Product and Process Description	Chloroacetic acid is a precursor for the production of amphoteric surfactants. Chloroacetic acid is produced by the catalyzed chlorination of acetic acid with chlorine. This process is characterized by its high selectivity. In the LCA model acetic anhydride is used as a catalyst as well as palladium on a carrier such as silica gel or carbon. The desired product, chloroacetic acid, is received in a product mixture of mono-, di- and trichloroacetic acid. Therefore the reaction mixture is treated by catalytic hydrogenation at elevated temperature to form chloroacetic acid. The resulting hydrogenchloride as a co-product is transformed into concentrated hydrochloric acid after purification [5].
Application	Chloroacetic acid is used in the manufacture of cellulose ethers (used mainly for drilling muds, detergents, food, and pharmaceuticals), as a post-emergence contact herbicide and defoliant, and in the manufacture of glycine and thioglycolic acid. Chloroacetic acid is also used in the manufacture of various dyes, synthetic caffeine, and organic chemicals.

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 Eco-profiles 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 Chloroacetic acid. Chloroacetic acid 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]

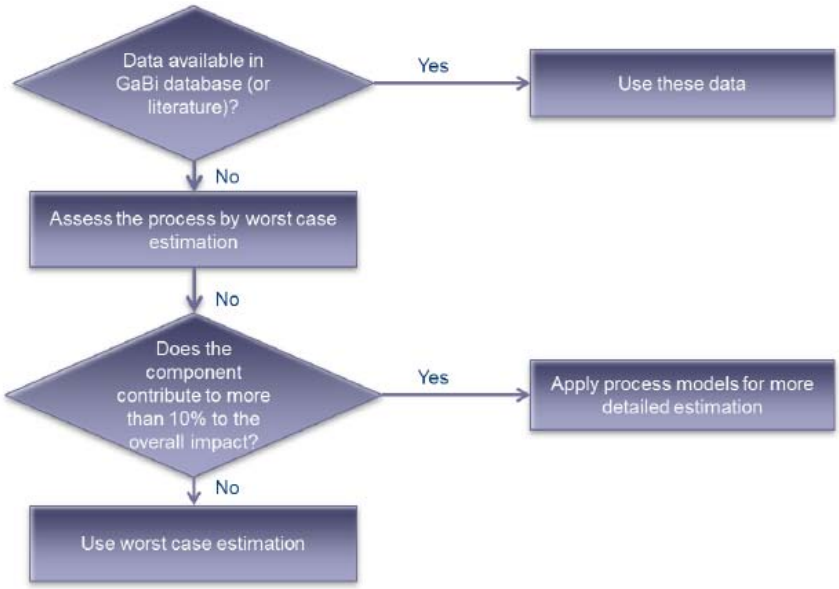
The main goal was to update the existing LCI inventories [3] for the production of Chloroacetic acid.

Temporal Coverage	Data collected for production refer to literature research covering recent production technology. The reference year was set up 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 Chloroacetic acid came from internal database and covers European conditions. The geographical representativeness for Chloroacetic acid was considered 'good'.
Technological Coverage	The technological representativeness for Chloroacetic acid was considered 'good'. Figure 1 provides a schematic overview of the production process of Chloroacetic acid.
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 Chloroacetic acid active substance.
Cradle-to Gate System Boundaries	

Included	Excluded
Chlorine production	Construction of major capital equipment (Infrastructure)
Acetic acid production	Maintenance and operation of support equipment
Acetic anhydride production	Human labor and employee transport
Dichloromethane production	Packaging
Energy production	
Utilities	
Transportation processes for the main materials	
Water use and treatment of waste water	
Treatment of wastes	

Assumptions and Limitations	The modelled data is according to stoichiometric amounts and based on secondary data from literature. The amount of catalyst is estimated by similar production processes. The amount of cooling water and energy were estimated using different methods: extrapolation, approximation with

similar chemicals, molecular structure-based models and process models following the recent production technology (cf. flowchart below).



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	The yield of the reaction was 72.9% of chloroacetic acid. The residual of 27.1% was the byproduct hydrochloric acid. Therefore an allocation by mass for 1 kg of the desired product chloroacetic acid was implemented in the model.
	Aggregated data	From public data and literature research.

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 PED impact is caused by acetic acid, chlorine and process steam as well as the catalyst acetic anhydride which contributes by 8% to the primary energy demand. The precursors acetic acid and chlorine represent the highest input by mass and contribute 43% and 34% to the total primary energy demand. Further, applied process steam contributes 11% to PED. The remaining contribution is due to electricity supply, use of catalyst, use of hydrogen, direct emissions, water use, waste and waste water treatment.

Global Warming Potential (GWP): An analysis of the inventory data shows that the GWP impact is caused by acetic acid, chlorine and process steam as well as the catalyst acetic anhydride which contributes by almost 8% to the global warming potential. The precursors acetic acid and chlorine represent the highest input by mass and 31% and 42% to the total impact of global warming potential. Further, applied process steam contributes 14% to GWP. The remaining contribution is due to electricity supply, use of catalyst, use of hydrogen, direct emissions, water use, waste and waste water treatment.

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

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	1573
Primary energy demand from fossil materials (net calorific value)	MJ	28221
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	29794
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-93.6
Carbon dioxide, fossil	kg	1368
Carbon dioxide, biotic	kg	91.2
Carbon dioxide, from land use, land use change and peat oxidation	kg	-
Methane	kg	2.99
Nitrous oxide (laughing gas)	kg	0.03
NMVOC emissions	kg	0.50
*Total GWP (according to [**IPCC 2007**])*	*t CO_2-equiv.*	*1.45*

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. [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, John Wiley & Sons, Inc., Hoboken, USA.

Figure 1. Production process of Chloroacetic Acid.