ERASM

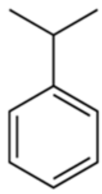
Date: 07/06/2016

Environmental Fact Sheet (#29)

Cumene

petrochemical surfactant precursor

Substance Identification

IUPAC Name	Isopropylbenzene	**CAS Number**	98-82-8
Other Names	Cumene; 2-Phenylpropane; Benzene, isopropyl; Propane, 2-phenyl		
Molecular Formula	C9H12	Structural formula: 	

Physical/Chemical Properties [1]

Molecular Weight	120.19 g/mol
Physical state	Liquid
Appearance	Clear liquid
Odour	Characteristic of aromatic compounds
Density	0.86 g/cm³ at 20°C
Melting Points	-96°C
Boiling point	152.39°C
Flash Point	31°C
Vapour Pressure	2.5 hPa at 25 °C
Water Solubility	Slightly soluble (0.1-100 mg/L)
Flammability	Flammable
Explosive Properties	Explosive (Lower explosive limit (EL): 0.9 vol%; Upper EL: 6.5 vol%)
Surface Tension	28.2 mN/m at 20°C
Octanol/water Partition coefficient (Kow)	log K_{OW} =3.55 at 23°C
Product and Process Description	Cumene is a surfactant precursor, which is used in this study for the production of the anionic surfactant sodium cumene sulphonate. Cumene is exclusively produced by alkylation of benzene. Therefore propene is reacted with benzene. For this gas phase alkylation process phosphoric acid on silica serves as a catalyst. The reaction is promoted by a Friedel-Crafts catalyst at about 200-250°C and 20- 40 bar. In the propene/propane mixture that is used other olefins should be very low concentrated. An excess of benzene is recommended to reduce further oligopropylation. Conversion is almost complete, but yet unreacted benzene and propane are distilled off the product stream and recycled. [5]
Application	Cumene is used for the production of phenol and acetone. It can also be used as a paint thinner, as a constituent for some petroleum-based solvents, and as a component of high-octane aviation fuel.

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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 cumene. Cumene 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/

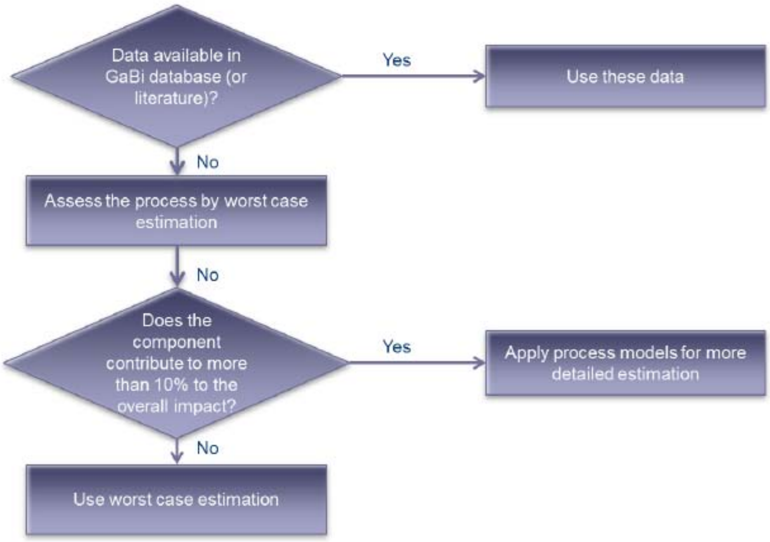
Goal and Scope of ERASM SLE project [2]

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

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 cumene came from internal database and covers European conditions. The geographical representativeness for cumene was considered 'very good'.
Technological Coverage	The technological representativeness for cumene was considered 'very good'. Figure 1 provides a schematic overview of the production process of cumene.
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 cumene active substance
Cradle-to Gate System Boundaries	see table below
Assumptions and Limitations	The present model for the production process of Cumene is based on literature [5]. The catalyst is neglected due to absence of relevant information. Energy as well as cooling water amounts 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).

Cradle-to Gate System Boundaries:

Included	Excluded
Propene production	Construction of major capital equipment (Infrastructure)
Benzene 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	

<table>
<tr><td></td><td colspan="2">
</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>No allocation was applied.</td></tr>
<tr><td>Aggregated data</td><td>From public data and literature research.</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): n analysis of the inventory data shows that the PED impact is caused by the raw materials benzene and propylene and the generation of process steam. The precursors, benzene and propylene, represent the highest input by mass and contribute 67% and 31%, respectively, to the total primary energy demand. Further the applied process steam contributes 2% to PED. The remaining contribution is due to electricity supply, 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 the raw materials benzene and propylene and the generation of process steam. The precursors, benzene and propylene, represent the highest input by mass and contribute 78% and 14% of the global warming potential. Further the applied process steam contributes 6% to GWP. The remaining contribution (2%) is due to electricity supply, 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 Cumene 100% active substance

LCI result	Unit	Amount
Primary energy demand		
Primary energy demand from renewable materials (net calorific value)	MJ	238
Primary energy demand from fossil materials (net calorific value)	MJ	59535
Primary energy demand from fossil and renewable materials (net calorific value)	MJ	59772
Air emissions related to Global Warming Potential		
Carbon uptake, biotic	kg CO_2 equiv.	-9.08
Carbon dioxide, fossil	kg	1090
Carbon dioxide, biotic	kg	10,4
Carbon dioxide, from land use and land use change	kg	-
Methane	kg	5.03
Nitrous oxide (laughing gas)	kg	0,0242
NMVOC emissions	kg	1.94
*Total GWP (according to [**IPCC 2007**])*	*t CO_2-equiv.*	*1.22*

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
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] Arpe H.-J. (2010). Industrial Organic Chemistry, 5th Edition, Wiley-VCH Verlag.

Figure 1. Production process of Cumene.