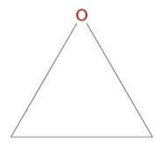
Date: 02/06/2017

# Environmental Fact Sheet (#8)

# Ethylene Oxide (EO)

## Petrochemical precursor

## Substance Identification

| | | | |
|---|---|---|---|
| **IUPAC Name** | Oxirane | **CAS Number** | 75-21-8 |
| **Other Names** | Ethylene oxide; Oxane; Dimethylene oxide; Oxiran; Ethene oxide. | | |
| **Molecular Formula** | $CH_2CH_2$0 | Structural formula:  | |

## Physical/Chemical Properties [1]

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|---|---|
| Molecular Weight | 44 g/mol |
| Physical state | Gaseous |
| Appearance | Colourless |
| Odour | Sweetish, ethereal |
| Density | Gas density:2.9 g/l at 20 °C<br>Liquid density:0.89 g/l at 10 °C |
| Melting Points | -112.5 °C |
| Boiling point | 10.7 °C at 101.3 kPa |
| Flash Point | -57 °C at 101.3 kPa |
| Vapour Pressure | 1456 hPa at 20°C |
| Water Solubility | Completely miscible in all proportions |
| Flammability | Gas: highly flammable and extremely reactive (exothermic reactions).<br>Aqueous solutions containing ethylene oxide are flammable or highly flammable. |
| Explosive Properties | Explosive |
| Surface Tension | 24.3 mN/m at 20°C |
| Octanol/water Partition coefficient (Kow) | log $K_{OW}$ = -0.3 (at 25°C) |
| Product and Process Description | Ethylene oxide is a reactive three-membered cyclic ether, widely used as surfactant precursor. Ethylene oxide is industrially produced by direct oxidation of ethylene in the presence of silver catalyst. The technologies are very similar, but differences exist, depending on whether air or pure oxygen is used for oxidation. All the industry data provided in this inventory indicated the use of oxygen for this process. The direct partial oxidation process is highly exothermic and is carefully controlled to minimize the total combustion of ethylene to carbon dioxide and water. Even so, 20-25% of the ethylene feedstock is typically lost via complete oxidation. The heat of reaction may be recovered by steam generation and used in other neighbouring processes. Aldehydes and glycols are typically obtained as co-products in the reaction process. [5] |
| Application | Ethylene oxide is widely used as surfactant precursor |

# 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 Ethylene Oxide (EO). EO is a petrochemical 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 [3,5] for the production of ethylene oxide.

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|---|---|
| Temporal Coverage | Data collected represents EO production of the year 2011; using yearly averages seasonal variations were balanced out. 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 were based on three suppliers representing EO production in Europe.<br>The geographical representativeness for EO was considered 'good'. |
| Technological Coverage | The technological representativeness for EO was considered 'very good'.<br>Figure 1 provides a schematic overview of the production process of EO. |
| Representativeness for market volume | >70% (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].<br>Functional Unit: 1 metric tonne of Ethylene Oxide 100% active substance. |
| Cradle-to Gate System Boundaries | (see table below) |
| Assumptions and Limitations | Mass- and impact-relevant catalysts and other chemicals were estimated by expert judgement, otherwise a cut-off was applied according to the given cut-off rules below.<br>Transportation was only considered for the main materials (covers about 90% of the mass of all inputs), other transportation was not considered. |
| Cut-off Criteria [4] | No significant cut-offs were used.<br>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.<br>The study included any material that had environmental significance in its extraction, manufacture, |

Cradle-to Gate System Boundaries:

| Included | Excluded |
|---|---|
| Ethylene production | Construction of major capital equipment (Infrastructure) |
| Oxygen 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 | |

| | | |
|---|---|---|
| | | 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 | Price allocation was applied to foreground system. The by-products of the ethylene oxide production are glycols and carbon dioxide. Especially carbon dioxide can be separated easily and is a by-product of low economic value compared to EO. Glycols are produced in very low quantities of the whole production output and can be sold for other applications. Besides, allocation was applied for some background data. |
| | 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 Ethylene Oxide 100% active substance**

| LCI result | Unit | Amount |
|---|---|---|
| **Primary energy demand** | | |
| Primary energy demand from renewable materials (net calorific value) | MJ | 938 |
| Primary energy demand from fossil materials (net calorific value) | MJ | 55596 |
| Primary energy demand from fossil and renewable materials (net calorific value) | MJ | 56535 |
| **Air emissions related to Global Warming Potential** | | |
| Carbon uptake, biotic | kg $CO_2$ equiv. | -50 |
| Carbon dioxide, fossil | kg | 1445 |
| Carbon dioxide, biotic | kg | 53 |
| Carbon dioxide, from land use, land use change and peat oxidation | kg | - |
| Methane | kg | 5.64 |
| Nitrous oxide (laughing gas) | kg | 0.03 |
| NMVOC emissions | kg | 1.39 |
| *Total GWP (according to [***IPCC 2007***])* | *t $CO_2$-equiv.* | *1.60* |

<u>Primary Energy Demand</u> (PED): An analysis of the inventory data showed that the main contributor is ethylene with 67% of the total, which has the highest input by mass. Oxygen is also one of the highest inputs by mass and requires ca. 9% of the total primary energy demand. Direct process emissions make up around 8% of the PED. Generation of electricity and thermal energy contribute 11% and 2% respectively to the PED. Utilities as cooling and process water as well as inert gas, transports and process waste treatment represent the remaining 3%.

<u>Global Warming Potential</u> (GWP): An analysis of the inventory data showed that the main contributor is ethylene with 67% of the total, which has the highest input by mass. Oxygen is also one of the highest inputs by mass and requires ca. 9% of the total global warming potential. Direct process emissions make up around 8% of the GWP. Generation of electricity and thermal energy contribute 11% and 2% respectively to the GWP. Utilities as cooling and process water as well as inert gas, transports and process waste treatment represent the remaining 3%.

| 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<br>Mrs. Charlotte Petiot and Dr. Yannick Leguern, BiolS by Deloitte |
| References | [1] ECHA. http://echa.europa.eu<br>[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.<br>[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<br>[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.<br>[5] Franke *et al.* (1995). A life-cycle inventory for the production of petrochemical intermediates in Europe. Tenside Surf. Det. 32, 384–396. |

Figure1. Production process of Ethylene Oxide.