EVALUATION OF POTENTIAL ENVIRONMENTAL EXPOSURE FOR PERFLUORINATED 8-2 TELOMER B ALCOHOL

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Introduction

Linear chain perfluorinated Telomer Alcohols are industrial chemicals occurring as intermediates in the manufacture of various polymeric materials containing fluorinated alkyl groups[1]. Telomer Alcohols are a raw material made from Telomer A and are used to manufacture polymeric products. The world-wide production of Telomer A has been estimated to be some 5,000 tons per year. Values for global production, use and environmental release of Telomer Alcohols are not yet available.[2] In this paper we apply three different multimedia models to exemplarily evaluate the environmental exposure, overall persistence (Pov) and long range transport potential (LRTP) of the perfluorinated 8-2 Telomer B Alcohol (8-2 TBA).

Multimedia Models and Simulation Scenarios

	SimpleBox [4]	ELPOS [5]	CliMoChem [6]
Characteristics	• Regional steady-state mass balance model • Part of EUSES	Steady-state mass balance model for the evaluation of Pov and LRTP	• Dynamic box model of 20 latitudinal coupled zones • Temperature effects
Scenario(s)	•Industrial textile application •Regional scale: Germany •Continental scale: EU	Complete emission into air, water or soil, respectively.	Heavily industrialized zones (6 and 7) as emission sources
8-2 TBA Emission	•One regional company •Eight on the continental level •Each emitting 475 kg/a into air and 25 kg/a into wastewater	• Generic emission scenario • Independent of total amount	• Singular pulse emission into air in each of the two zones
Output	•Steady-state concentrations •Mass distribution •Sensitivity (with Crystal Ball®)	•Characteristic travel distance (CTD) •Overall persistence (Pov)	• Zonal concentration dynamics in air, sea and soil • Mass distributions and fluxes

Substance data of 8-2 TBA [2]

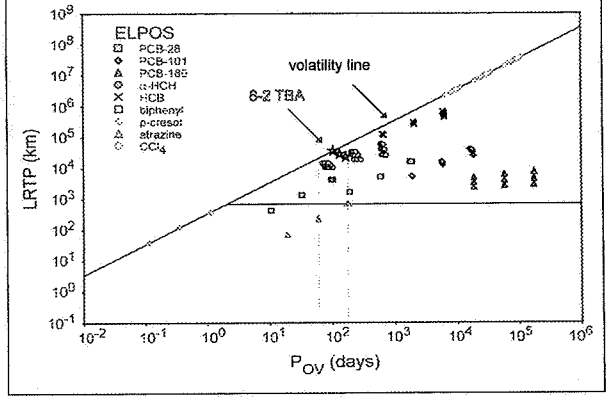
CAS No.	678-39-7
molar mass	464.11
m.p.	42 – 44°C
vapor pressure	3 Pa (20°C)
water solubility	0.137 ± 0.053 mg/L
K_{AW} (calculated)	3 – 6.7
ΔH_{vap} (estimated)	20 – 40 kJ/mol
log K_{OW}	4.5 – 5.3
log K_{OC} (calc. from K_{OW})	4.0 – 4.9
$t_{½}$ in air	6 – 16 d [7]

SimpleBox Results

	Air	Water	Sediment	Soil
mass fraction	55 – 70%	< 1%	< 1%	30 – 45%
regional concentration	20 – 30 pg/m³	0.5 – 1.0 pg/L	800 – 950 pg/kg	70 – 100 pg/kg
continental concentration	15 – 25 pg/m³	0.3 – 0.7 pg/L	500 – 650 pg/kg	80 – 110 pg/kg
C.V. of regional concentration	10 – 15 %	15 – 20%	80 – 90%	90 – 100%
most sensitive parameters	$t_{½}$ in air, advective flow	STP parameter, K_{OC}, K_{AW}	K_{OC}	K_{OC}, K_{AW}

ELPOS Result

Max. LRTP vs. max. P_{OV} for 8-2 TBA and a set of well-known reference chemicals



SimpleBox - Sensitivity Analysis

To identify the most sensitive parameters a probabilistic simulation is performed by coupling SimpleBox with Crystal Ball® software[3]. For this purpose information about uncertain input parameters is translated into frequency distributions around the most probable value. Substance parameters K_{AW} and K_{OC} showed highest sensitivity. Except for air concentration the K_{OC}, which is meant to describe the sorption to surface media (soil and sediment), proved to be of high sensitivity. The large coefficients of variation for soil and sediment concentration are a direct effect of the uncertainty of the K_{OC}. It is thus necessary to get a more accurate quantitative description for the sorption and volatilization behavior of 8-2 TBA to get a better basis for future modeling. Respective experiments have been initiated with a cooperation partner.

CliMoChem Results

Preliminary simulations with CliMoChem on the basis of available substance data indicate a potential for transport of 8-2 TBA to arctic regions. Air concentration of 8-2 TBA one year after pulse emission in temperate zones is highest in the arctic (zone 1). The concentration ratio between air and soil decreases by a factor of about 1.2 from the emission zones (temperate zones 6 and 7) to northern polar zone 2 indicating a low potential for cold condensation. Total accumulated mass in northern zones (1 and 2) is low due to the high volatility and small atmospheric lifetime.

Discussion

Simulated steady-state concentrations of 8-2 TBA for a textile application emission scenario have been calculated with SimpleBox. Total substance mass is estimated to mainly reside in air compartment (55 – 70%). Due to the model structure emissions into wastewater lead to accumulation in sewage sludge and subsequent sludge application to agricultural soil explains the calculated mass fraction of 30 – 45 % in the soil compartment.

Long range transport potential of 8-2 TBA as calculated with ELPOS is intermediate compared to some well known reference chemicals.

Preliminary results from CliMoChem model, which are based on available data being currently refined, suggest a potential for transport to arctic regions, but indicate a low potential for cold condensation in these zones.

Acknowledgements

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