Society of Environmental Toxicology & Chemistry
Summary of DuPont Presentations

North American World Congress
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Biotransformation of ^{14}C-labeled Fluorotelomer substances by microorganisms from activated sludge or soil.
Wang, N[1], Szostek, B[2], Buck, R[3], Folsom, P, Sulecki, L[1], Gannon, J[1], [1] DuPont Central Research and Development, Newark, DE, USA[2] DuPont Haskell Laboratory for Health and Environmental Sciences, Newark, DE, USA[3] DuPont Chemical Solutions Enterprise, Wilmington, DE, USA
ABSTRACT- The environmental fate of chemicals containing perfluorocarbon moieties [F(CF_2)n-] is of increasing scientific and public interest. The perfluorocarbon moieties, such as 8-2 Telomer B alcohol [$F(CF_2)_8CH_2CH_2OH$], are building blocks of fluorotelomer-based consumer products. As part of environmental stewardship effort, we are investigating the biodegradation potential and possible biotransformation pathways of fluorotelomer products by activated sludge or by soil microorganisms. To unequivocally identify transformation products and to achieve mass balance of the test materials, ^{14}C-labeled 8-2 Telomer B Alcohol ([$F(CF_2)_7{}^{14}CF_2CH_2CH_2OH$] and ^{14}C-labeled fluorotelomer poly urethane were custom synthesized and were used for the study. The experimental methods, bioavailability of the test materials, observed transformation products, and potential biotransofrmation pathways will be discussed. The potential for microbial defluorination of perfluorinated C-C bonds of the test materials will also be discussed.

The Fate of Fluorotelomer Treated Consumer Articles in a Municipal Waste Incinerator.
Taylor, P[1], Yamada, T[1], Giraud, R[2], Kaiser, M[2], Buck, R[2], [1] University of Dayton Research Institute, Environmental Engineering Group, Dayton, OH, USA[2] E. I. du Pont de Nemours & Co., Inc., Wilmington, DE, USA
ABSTRACT- The fate of fluorinated substances in the environment and their routes into the environment are areas of regulatory, industrial and academic interest. Textiles and paper are often incinerated when they are disposed. No information regarding emissions from incineration of textiles or paper treated with fluorotelomer-based products is available. This paper reports the first known studies to investigate the thermal degradation behavior of a fabric treated with a fluorotelomer-based acrylic polymer under laboratory conditions conservatively representing typical municipal incineration conditions of time, temperature, and excess air level. Additional laboratory-scale non-flame thermal degradation studies from 600 to 1000 degrees C for gas-phase residence times of 2.0 seconds were conducted to establish the temperature at which 99.9% destruction was achieved. Carbon mass balance was achieved. The thermal reactor effluent was analyzed by in-line GC/MS to identify degradation products. The details of the experimental procedures and results will be presented.

Comparative Acute Toxicity of Three Fluorotelomer Acids to *Pseudokirchneriella subcapitata, Daphnia magna*, and *Oncorhynchus mykiss*.
Hoke, R.[1], Bouchelle, L.[1], Ferrell, B.[1], Buck, R.[2], [1] DuPont, Haskell Laboratory for Health and Environmental Sciences, Newark, DE, USA[2] DuPont, Wilmington, DE, USA
ABSTRACT- Perfluorinated compounds have unique properties and their measurement in various environmental matrices has received increased attention. While PFOS and PFOA have been the focus of much of this attention, fluorotelomer alcohols and acids have also been of interest. We conducted 48, 72 and 96-hour aquatic toxicity tests to evaluate the toxicity of three fluorotelomer acids to the cladoceran, *Daphnia magna*, the green alga, *Pseudokirchneriella subcapitata*, and the rainbow trout, *Oncorhynchus mykiss*, as part of an on-going product stewardship program. The three fluorotelomer acids tested were 2-perfluorooctyl ethanoic acid, 2H-hexadecafluoro-2-decenoic acid, and n-perfluorodecanoic acid. The cladoceran, *Daphnia magna*, was generally the most sensitive species tested followed by the green alga, *Pseudokirchneriella subcapitata*. Rainbow trout were generally less sensitive to the fluorotelomer acids than the other test species. These results suggest that the acute toxicity of these fluorotelomer acids is of low to medium concern from a hazard classification standpoint. When coupled with potential environmental exposure concentrations, these data suggest that the fluorotelomer acids tested pose little risk for acute aquatic toxicity in the environment.

Comparative Toxicity of Two Fluorotelomer-based Surfactants to the Green Alga, *Pseudokirchneriella subcapitata*.
Sloman, T.[1], Hoke, R.[1], Szostek, B.[1], Ferrell, B.[1], Prickett, K.[1], Buck, R.[2], [1] DuPont, Haskell Laboratory for Health and Environmental Sciences, Newark, DE, USA[2] DuPont, Wilmington, DE

ABSTRACT- Perfluorinated compounds have unique properties and their measurement in various environmental matrices has received increased attention. Their unique properties and use as surfactants, with accompanying potential for environmental release, make aquatic hazard assessment an integral part of product stewardship and risk assessment. The green alga, *Pseudokirchneriella subcapitata,* (aka *Selenastrum capricornutum*) was exposed for 72 hours to each of two fluorotelomer-based surfactants; one anionic and the other nonionic, in regulatory guideline studies conducted using Good Laboratory Practices to assess the potential aquatic hazard of each compound to algae. The 72-hour EC50s based on inhibition of healthy cell count, area under the growth curve, and growth rate were greater than 100 mg/L for both compounds. The lowest 72-hour NOEC for the anionic surfactant was 25 mg/L while the 72-hour NOEC for the nonionic surfactant was 100 mg/L.

Comparative Early Life Stage Toxicity of Two Fluorotelomer-based Surfactants Using Rainbow Trout.
Hoke, R.[1], Turner, Sr., J.[1], Szostek, B.[1], Bouchelle, L.[1], Ferrell, B.[1], Prickett, K.[1], Buck, R.[2], [1] DuPont, Haskell Laboratory for Health and Environmental Sciences, Newark, DE, USA[2] DuPont, Wilmington, DE, USA
ABSTRACT- Perfluorinated compounds have received increased attention because of their unique properties and measurement in various environmental matrices. Their unique properties and use as surfactants, with accompanying potential for environmental release, makes aquatic hazard assessment an integral part of product stewardship and risk assessment. Acute and chronic toxicity tests were performed with fish to assess the aquatic hazard of two fluorotelomer-based surfactants; one anionic and the other nonionic. Non-GLP acute screening studies and GLP rainbow trout early-life stage toxicity tests conducted according to regulatory guideline methods were used to assess the toxicity of both surfactants. The results of the acute and chronic hazard testing are presented along with illustrations of the novel challenges presented in the aquatic toxicity testing and associated chemical analysis of these compounds.

Bacterial Respiration Inhibition Studies of Fluorotelomer-Based Products.
Berti, William[1], Wang, Ning[1], Sulecki, Lisa[1], Folsom, Patrick[1], Buck, Robert[2], [1] DuPont Central Research & Development, Newark, DE, USA[2] DuPont Chemical Solutions Enterprise, Wilmington, DE, USA
ABSTRACT- Fluorotelomer-based products provide unique properties to a wide variety of consumer goods. These products may find their way into wastewater treatment plants through normal use and disposal. Bacterial respiration inhibition studies help estimate the effect of the test material on mixed communities of bacteria in aquatic environments, especially in aerobic biological treatment systems. These studies also can be useful to help determine test concentrations to use in biodegradation studies. We studied the inhibition to bacterial growth in activated sludge of municipal wastewater treatment facilities using both guideline and non-guideline methods for a series of fluorotelomer-based products. At the highest test concentration at which they were dosed, 1000 mg L^{-1}, the test substances exhibited no respiration inhibition. The EC_{50}, which is the effective concentration of the test material resulting in a 50% calculated or interpolated inhibition of oxygen consumption compared with a control blank, are estimated to be greater than 1000 mg L^{-1}.

Matrix-effect free analytical methods for determination of perfluorinated carboxylic acids in environmental and biological samples.
Powley, C[1], Ryan, T[1], George, S[1], [1] DuPont Haskell Laboratories, Newark, DE, USA
ABSTRACT- The sample matrix can often have significant effects upon the performance of analytical methods for the quantitative determination of perfluorinated carboxylic acids in environmental and biological samples. These effects can include inhibition of the extraction procedure due to binding of residues and suppression or enhancement of the signal obtained in LC/MS/MS determinations. We have developed methods for the determination of perfluorinated carboxylic acids in environmental matrices (soil, sediment and sludge) that address these issues, with limits of quantitation of 1 ppb. Extraction efficiency is demonstrated with fortifications prepared using a procedure that mimics field weathering of the residues. Matrix enhancement and suppression are reduced to a negligible extent using isotopically-labeled internal standards when these analogs are available and novel solid-phase extraction (SPE) procedures when they are not. The same procedures are used to purify extracts from biological matrices with similar success, with limit of quantitation of 1-5 ppb. Quality control data have been developed that demonstrates (1) recovery of laboratory fortifications; (2) freedom from matrix enhancement or suppression; (3) recovery of aged residues and (4) absence of significant background interference.

The Role of Photolysis in the Atmospheric Fate of Perfluorinated Aldehydes: Gas Phase UV and IR Absorption Spectra.

Society of Environmental Toxicology & Chemistry
Summary of DuPont Presentations

Hashikawa, Y[1], Kawasaki, M[1], Sulbaek Andersen, M[2], Nielsen, O[2], Hurley, M[3], Wallington, T[3], Waterland, R[4], [1] Kyoto University, Kyoto, Japan[2] University of Copenhagen, Copenhagen, Denmark[3] Ford Motor Company, Dearborn, MI, USA[4] E. I. du Pont de Nemours & Co., Inc., Wilmington, DE, USA

ABSTRACT- Long-chain perfluoroalkyl carboxylic acids (PFCAs, $C_xF_{2x+1}COOH$, where x = 6 - 12) have been observed in remote locations and are presumed to be the atmospheric degradation products of precursor chemicals. Atmospheric oxidation of fluorotelomer alcohols (FTOHs), $C_xF_{2x+1}CH_2CH_2OH$, has been suggested as a possible source of PFCAs. It is well established that the initial atmospheric oxidation products of FTOHs are perfluorinated aldehydes, but the subsequent fate of these aldehydes is unclear at this time. Since UV photolysis is likely to be an important removal process for perfluorinated aldehydes, we have examined the UV and IR spectra of $C_xF_{2x+1}CHO$ (x=1-4) using computational and experimental techniques. We compare our results with the limited existing literature data and we discuss the relevance of these results to the atmospheric fate of $C_xF_{2x+1}CHO$.

SETAC Europe
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Perfluorooctyl Ethanol Biodegradation : Transformation Products and Pathway

Buck R.C.[1], Wang N.[2], Folsom P.W.[2], Szostek B.[3], Capka V.[3],and Gannon J.T.[2]; [1] DuPont Chemical Solutions Enterprise, Wilmington, DE, USA[2] DuPont Central Research and Development; USA [3] DuPont Haskell Laboratory, USA.

The environmental fate of chemicals containing perfluorocarbon moieties [$F(CF_2)_n$-] is of increasing scientific and public interest. Carbon-fluorine bonds are extremely strong (116 kcal•mol^{-1}). As a result, it is generally believed that perfluorocarbon chains do not readily biodegrade and carbon-carbon bond scission in the perfluorocarbon chain is not expected. We have investigated the biotransformation in microbial culture of radiolabeled perfluorooctyl ethanol, $F(CF_2)_7{}^{14}CF_2CH_2CH_2OH$, commonly known as 8-2 Telomer B Alcohol, under a number of conditions and timeframes to elucidate the biotransformation pathway(s) and identify transformation products. The studies conducted, including major transformation products and proposed transformation pathway(s), will be discussed. The results demonstrate that the $-CH_2CH_2-$ "spacer" influences the biotransformation pathway(s). Among many metabolites observed, $F(CF_2)_7COOH$ is neither the major nor the final stable biotransformation product.

Soil-Water Partitioning of a Fluorotelomer Intermediate used to Manufacture Fluorotelomer-based Polymers

William R. Berti[1], Robert C. Buck[1], Hiroyuki Iwai[2], Ning Wang[1], Volker Koch[3], Seiji Shinya[4], Bogden Szostek[1], Robert Waterland[1] - Telomer Research Program
[1]DuPont Co., [2]Daikin Industries, Ltd., [3]Clariant GmbH, [4]Asahi Glass Co., Ltd.

Fluorotelomer intermediates are used to manufacture fluorotelomer-based polymer products, which provide unique properties to a wide variety of consumer products. Four telomer manufacturers that are collectively sponsoring research on telomer compounds jointly sponsor the Telomer Research Program (TRP). The TRP program includes investigations on the environmental fate and effects properties of fluorotelomer intermediates. A soil-water partitioning study using a batch equilibrium method is being conducted on the fluorotelomer intermediate 8-2 Telomer B Alcohol [8-2 TBA; $CF_3(CF_2)_7CH_2CH_2OH$, CAS# 678-39-7]. Results of the study demonstrated that greater than 90% of ^{14}C-labelled 8-2 TBA initially added to the test system partitioned to soil and sediment within three hours. The 8-2 TBA partitioned to activated sludge within one hour. Less than 2% remained in the aqueous phase at a 1:1 soil:solution ratio after 3 hours at 4°C; total recovery of the compound was 95% and greater under these conditions. In one soil after 24 h equilibration time and at room temperature, 50% or more of the ^{14}C label added as 8-2 TBA was bound to the residual fraction, which was determined by combusting the soil after three washings with acetone, air-drying, and grinding. We will summarize the soil-water partitioning studies that have been conducted on the 8-2 TBA, including adsorption and desorption isotherm data and the organic carbon partitioning coefficients (Koc) determined in the studies. We will also discuss progress in understanding partitioning/ condensation of 8-2 TBA in the vapor phase to solids.

Physicochemical Properties of Fluorotelomer Alcohols

Mary A. Kaiser,[1] Daryl P. Cobranchi,[1] Chien-Ping Chai Kao,[2] Paul J. Krusic,[3] Alexander A. Marchione,[3] and Robert C. Buck[4]

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Physicochemical properties such as vapor pressure and solubility are necessary to determine environmental transport potential and environmental fate. Often these properties are estimated from models based on properties of chemically similar materials. Fluorinated compounds, however, are especially difficult to model since the properties of fluorinated compounds are quite different from their hydrocarbon analogues. Fluorotelomer alcohols are also difficult to obtain in pure form since they are "products by process" which are a mixture of several compounds each differing by two carbon units.

This presentation describes three experiments used to measure vapor pressure of individual fluorotelomer alcohols, including a novel experiment using gas-phase nuclear magnetic resonance spectroscopy. The physicochemical properties of the fluorotelomer alcohols are compared to their hydrocarbon analogues to demonstrate their unusual properties.

Effects of Fluorotelomer Products on the Bacterial Growth, Degradation of Organic substances, and Microcosmic Population from Activated Sludge of Domestic Sewage Treatment Plant

Wang N.[1], Folsom P.W. [1], Decarolis, J., Berti W.R.[1], Buck R.C. [2], and Gannon, J.T. [1]. [1] DuPont Central Research and Development, Newark, DE, USA; [2] DuPont Chemical Solutions Enterprise, Wilmington, DE, USA.

Fluorotelomer-based materials are widely used in various consumer products. As part of environmental stewardship effort, we are investigating possible physiological impact of fluorotelomer-based products such as Zonyl 8300, Zonyl FCC, Zonyl FSN and Zonyl FSP on the microcosm from activated sludge of domestic sewage treatment plant (POTW). The growth of bacteria at the presence of up to 1g TOC-equivalent L^{-1} of the fluorotelomer products in addition to 0.1% yeast extract was monitored by measuring the turbidity (absorbance at 600 nm) for 48 h at 30 °C. The growth patterns of the bacteria were very similar at the presence or absence of the fluorotelomer products and none of the products showed any inhibitory effect on the bacterial growth at the highest product concentration (1g TOC-equivalent L^{-1}). The ability of the activated sludge to degrade organic substances such as ^{14}C-labeled aniline at the presence of fluorotelomer products will be discussed. The results about the impact of the fluorotelomer products on the microcosmic population (monitored over time by denatured gradient gel electrophoresis) will also be presented.

Application of LC-MS/MS methodology to determination of Telomer B alcohols, perfluorinated acids, and fluorosurfactants in environmental matrices.

Bogdan Szostek[1], Vladimir Capka[1], Keith B. Prickett[1], S. Mark Kennedy[1], Robert C. Buck[2]

1. DuPont Haskell Laboratory for Health and Environmental Sciences, Newark, DE
2. DuPont Chemical Solutions Enterprise, Wilmington, DE, USA

A need for measurement of perfluorinated compounds in environmental matrices has increased significantly in recent years. Appropriate analytical methodology, sampling, sample preparation procedures, as well as applicable measurement techniques are being established by many researchers for this group of compounds. Unique physico-chemical properties of these compounds require special consideration when analytical methods are established. Especially, a careful method validation demonstrating proper spike recoveries for the matrix of interest, "clean" blanks, and sample storage conditions are of the most importance.

Our effort is focused around the development of analytical methodology for Telomer B alcohols, biodegradation products of Telomer B alcohols, Telomer-derived fluorosurfactants, and polymers in environmental matrices to support environmental fate and effects studies with these materials. LC-MS/MS methodology is predominantly utilized for determination of perfluorinated acids. GC-MS methodology has been traditionally utilized for determination of telomer B alcohols. There is a strong demand to be able to measure both of these types of analytes by a single technique. The presentation will discuss our efforts to measure both types of analytes by LC-MS/MS. Appropriate sample preparation, clean-up procedures, samples storage conditions, method validation data, achievable limit of detection, and analyte specific recommendations will be discussed. Additionally, challenges of analyzing complex mixtures of fluorosurfactants and applicable analytical methodology will be outlined.

TELOMER RESEARCH PROGRAM

Ecotoxicity Profile of 1H,1H,2H,2H-Perfluorodecanol (C8-2 Telomer B Alcohol)

Volker Koch[1], William R Berti[2], Robert C Buck[2], John Gannon[2], Robert A Hoke[2], Hiroyuki Iwai[3], Mary A Kaiser[2], Seiji Shinya[4], Ning Wang[2] – Telomer Research Program

[1]Clariant Germany, [2]DuPont USA, [3]Daikin Japan, [4]Ashai Glass Japan

1H,1H,2H,2H-Perfluorodecanol, CAS No. 678-39-7 (C8-2 Telomer B Alcohol) is an important speciality intermediate. More than 80% of the produced amount of telomer alcohols are used for the preparation of high

molecular weight polyacrylate polymers containing perfluorinated alcohols. These so-called Telomer-based Polyacrylate Polymers (TBPPs) are used e.g. for the coating of textiles and carpets to achieve resistance against water, oil and stains.

The producers of telomer alcohols are currently investigating in detail the environmental fate and effects properties of telomer alcohols and especially of 1H,1H,2H,2H-Perfluorodecanol within the Telomer Research Program (TRP).

Telomer alcohols have in comparison to their hydrogenated counterparts exceptional physico-chemical properties which are related to the fluorine atoms. But these properties (e.g. very low water solubility, high vapour pressure) are considerable challenges for ecotoxicity testing. Within TRP testing strategies for this substance which is difficult to test were developed based on state-of-the-art methodology.

The poster will present basic physico-chemical properties of 1H,1H,2H,2H-Perfluorodecanol, applied design for acute and chronic aquatic tests as well as terrestrial / sediment tests and the results for the different species tested.

Evaluation of Environmental Exposure and Long-range Tranport Potential for Perfluorinated 8-2 Telomer B Alcohol

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Available substance data of perfluorinated 8-2 Telomer B Alcohol (8-2 TBA) have been evaluated and necessary input data for model calculations have been compiled. Data basis proved to be insufficient as some key parameters like K_{AW} and K_{OC} are highly uncertain. Assuming a realistic emission scenario for textile application [1] steady state concentrations have been estimated with SimpleBox multimedia model. More than 95% of total 8-2 TBA mass are calculated to reside in compartments air and agricultural soil. Steady state mass ratio between these two compartments proved to be strongly dependent on partitioning behavior expressed by K_{AW} and K_{OC}. For most combinations of these two parameters, mass fraction in air accounts to more than 60%. For sensitivity analyses probability distributions have been attributed to uncertain parameters and a Monte-Carlo analysis has been used to propagate these uncertainties through the model. Highest sensitivity is calculated for partition coefficients K_{AW} and K_{OC} affecting all compartments but air. Instead, air concentration is influenced by degradation rate in air, advective flow (wind speed) and respective emissions. Concentration in water is generally low and mostly dependent on emission assumptions. Characteristic travel distances (CTD) in air calculated with ELPOS multimedia model [2] is predominately determined by degradation in air, because deposition of the substance is considerably low. Ranking against a set of about 700 well-known environmental contaminants representing a wide variety of substance properties gave a rank coefficient of about 0.9 indicating a relatively high long range transport potential in air. Potential for condensation in cold regions is low. Average half-life in air is small (6 - 16 days [3]) compared to the average exchange time between troposphere and lower stratosphere (15-18 months) indicating that 8-2 TBA will not constitute a similar stratospheric problem like fluorinated hydrocarbons.

[1] Telomers Research Program, pers. communication, 2003.
[2] Beyer A., Matthies M.; *Criteria for atmospheric long-range transport potential and persistence of pesticides and industrial chemicals.* UBA-report no. 8/02, E. Schmidt Verlag Berlin, 2002
[3] Ellis D.A., Martin J.W., Mabury S.A., Hurley M.D., Andersen M.P.S., Wallington T.J.; *Environ. Sci. Technol.* **37 (17),** 3816-3820, 2003.

ATMOSPHERIC LIFETIMES AND DEGRADATION MECHANISMS OF FLUOROTELOMER ALCOHOLS CF3(CF2)nCH2CH2OH

Dr. Georges LeBras, CNRS-LCSR (Orléans, France)

Perfluorooctane sulfonate (PFOS) detected in humans and animals is very likely produced from polyfluorinated sulfonamido-ethanols. For this reason PFOS and related compounds have been phased out. The fluorotelomers alcohols (FTOHs) are mainly used in analogous polymeric applications as the sulfonamido-ethanols and they are expected to be present in the atmospheric gas phase.

In order to assess the environmental impact of FTOHs a kinetic and mechanistic study of the gas phase oxidation of such compounds by the OH radical has been carried out. The studied compounds are trifluoropropanol, CF3CH2CH2OH (TFP) and tridecafluorooctanol, C6F13CH2CH2OH (TDO).

The rate constant measurements of the OH reaction with TFP and TDO has provided similar values. This indicates that the length of the perfluorinated chain has no influence on the reactivity of the alcohol. Therefore the same rate constant can be recommended for larger FTOHs, such as 2-perfluoro-n-octyl ethanol, C8F17CH2CH2OH (2POE), which is of more industrial interest but difficult to investigate due to its low vapor pressure. The atmospheric lifetime of FTOHs deduced from the rate constant measurements is 11days.

The mechanistic study has been carried out in two photoreactors: a 150 L Teflon® bag irradiated by lamps and the 200 m3 European photoreactor irradiated by sunlight in Valencia (Spain). For the OH-initiated oxidation of TFP in air the major primary products are the fluoroaldehydes CF3CH2CHO and CF3CHO, in the presence and absence of NOx, CF2O being the end product. This mechanism can be generalised for larger FTOHs, including TDO and 2POE. In this case the intermediate aldehydes will be CF3(CH2)nCH2CHO and CF3(CF2)nCHO.

Based on the obtained data the amospheric fate of the FTOHs will be discussed.

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Development of analytical methodology for determination of Telomer B alcohols, Telomer-derived anionic, nonionic fluorosurfactants, and polymers.

Bogdan Szostek, Keith B. Prickett, Janet C. Maslanka, S. Mark Kennedy
DuPont Haskell Laboratory for Health and Environmental Sciences, Newark, DE

Telomer B Alcohols are intermediates in the manufacture of broad range of anionic and nonionic fluorosurfactants and polymers. Analytical methodology for determination of the Telomer B alcohols and Telomer-derived fluorosurfactants and polymers in environmental matrices is not well established. The presentation will discuss determination of Telomer B Alcohols by GC-MS and LC-MS techniques in environmental matrices. In addition, Telomer-based fluorosurfactants are complex multi-component mixtures of chemical species that possess no chromophores making traditional spectroscopic detection for LC separations not feasible. Determination of individual components of fluorosurfactants poses challenging analytical problem in respect to separation, detection, and quantitation. Two classes of fluorosurfactants will be discussed: anionic fluoroalkylphosphate surfactant and non-ionic ethoxylate fluorosurfactant. The presentation will describe our investigation of these two groups of fluorosurfactants mainly by liquid chromatography-mass spectrometry. Chromatographic separation of the components of these complex mixtures, their identification, establishment of figures of merit for mass spectrometric detection, and development of analytical methodology for analysis in aqueous matrices will be discussed. Also, analytical methodology suitable for determination of two types of Telomer-containing polymers: acrylate and urethane in environmental matrices will be presented.

Biotransformation of the ^{14}C-labeled fluorotelomer 8-2 Telomer B Alcohol (8-2 TBA)

Wang N.[1], Folsom P.W. [1] Berti W.R.[1], Szostek B.[2], Sulecki L.M., Capka V.[2], Gannon J.T.[1], and Buck R.C.[3]
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The 8-2 Telomer B Alcohol [$F(CF_2)_8CH_2CH_2OH$; CAS # 678-39-7] is a key raw material and intermediate used in the manufacture of sales products such as telomer-based fluorinated surfactants and polymers. Using ^{14}C-labeled 8-2 TBA, we have investigated the biodegradation potential and transformation products of this substance with microcosms from a POTW and an industrial wastewater treatment facility. The details of the test systems, substance handling, sample preparation, analytical methods, and the results of the biotransformation studies under various test conditions will be discussed.

Early-Life Stage Toxicity Testing of Fluorotelomer-based Surfactants Using Rainbow Trout, *Oncorhynchus mykiss*.

Hoke, R.A., Szostek, B., Turner, J.T., Sr., Bouchelle, L.D., Ferrell, B.D., Prickett, K.B. and Buck, R.C.

Fluorotelomer surfactants are an important class of industrial specialty chemicals because of their unique properties. They provide superior wetting action compared to non-fluorinated surfactants and are stable in harsh chemical and thermal environments. Their unique properties and use as surfactants, with accompanying potential for environmental release, makes aquatic hazard assessment an integral part of product stewardship and risk assessment. Acute and chronic toxicity tests were performed with fish to assess the aquatic hazard of two fluorotelomer-based surfactants; one anionic and the other nonionic. Non-GLP acute screening studies and GLP rainbow trout early-life stage studies conducted according to regulatory test methods were used to assess the toxicity of both surfactants. The results of the acute and chronic hazard testing are presented along with illustrations of the novel challenges presented in the aquatic toxicity testing and associated chemical analysis of these compounds.

Bioconcentration Screening of Fluorinated Compounds Using Fathead Minnows.

Hoke, R., Gibson, W.R., Good, R.M. and Buck, R.C.

Perfluorinated compounds have been the a focus interest for regulatory agencies and the industries that manufacture these compounds. The unique properties of many of these compounds have raised questions about their potential environmental stability and resulting effects, including the potential for bioaccumulation in fish. Regulatory bioconcentration testing is expensive and resource intensive, therefore, an initial evaluation of potential bioconcentration of several perfluorinated compounds in fish was conducted using a screening test design and total fluoride analysis of whole fish. Compounds evaluated included a positive control (an electrochemical fluorination-derived perfluorinated sulfonate), a fluorotelomer intermediate, a fluorotelomer polymer, and two fluorotelomer surfactants; one anionic and the other nonionic. The compounds were evaluated at a single concentration in a study composed of a 15-day uptake phase and a 14-day depuration phase. The unique challenges associated with screening the bioconcentration potential of these compounds and results are presented along with a discussion of the potential implications of the results for risk assessment.

Biodegradation studies of fluorotelomer-based surfactant and polymer products.

W.R. Berti[1], N. Wang[1], B. Szostek[3], S.M. Kennedy[3], J.T. Gannon[1], and R.C. Buck[2]

Fluorotelomer-based surfactant and polymer products provide unique properties to a wide variety of consumer products. We are studying their environmental fate by testing their potential to biodegrade using microbial inoculum from soil and from activated sludge of municipal waste-water treatment facilities. Carbon dioxide evolution, disappearance of dissolved oxygen, or disappearance of dissolved organic carbon from the liquid phase are being used as surrogate measurements to monitor changes in the test materials (i.e., the fluorotelomer-based surfactant or polymer products) during the course of the experiments. Fluoride concentrations are periodically measured in the test solutions to assess defluorination of the parent material. Results indicate that for the two surfactant products, the composition of which includes hydrocarbons, about 50% and 85% of the total carbon measured in the parent materials mineralized to CO_2. For polymer products used in the tests, less than 20% of the total carbon measured in the products mineralized. The production of CO_2 from the polymer products was most likely from the hydrocarbon surfactants used to disperse them in water. No significant fluoride production (<0.8% of the measured total) was observed in any of the tests to date. We are analyzing test solutions collected during the studies to determine what, if any, transformation products have been formed. The chemical analyses will focus on the possible production of fluorinated acids.

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Biotransformation of the fluorotelomer 8-2 Telomer B Alcohol (8-2 TBA) in bacterial culture

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The 8-2 Telomer B Alcohol [$F(CF_2)_8CH_2CH_2OH$; CAS # 678-39-7] is a primary raw material and intermediate used in the synthesis of various telomer-based fluorinated surfactants and polymers which are used in a wide range of consumer products. This compound is postulated to be an environmental degradation product arising from telomer-based fluorinated surfactants and polymers. We have investigated the biodegradation of this substance to determine whether or not it is environmentally persistent and if metabolic pathways are available for its further biotransformation to other fluorinated species. The 8-2 Telomer B Alcohol is surface active, sorptive to certain surfaces, of low solubility in water and may be volatile. As such, test systems and sampling and analysis methods have been carefully established for these studies. Biotransformation with adapted and unadapted sludge cell cultures under modified aerobic ready and accelerated conditions have been investigated and analysis of transformation products conducted. The details of the test systems, substance handling and the results of the biotransformation studies under a range of test conditions will be discussed.

Title: Perfluoroalkylated Substances in the Environment: What are they? Where to the come from? Where do they go? and What do we know about them?

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Abstract
Perfluoroalkylated substances (PFAS) are specialty materials utilized in a wide variety of end-use applications which take advantage of the unique properties of the perfluoroalkyl functionality. These substances are manufactured by different processes and have functionality differences that influence their performance, toxicological and environmental behavior. To start, this paper will begin by reviewing the "classes" of PFAS and then proceed to discuss how these substances are used, their routes into the environment via these uses and provide an overview of what is known about their environmental toxicology and fate. Although only a limited number of essential physicochemical data are available, thus hampering a complete assessment of the environmental fate of PFAS, it has become clear that PFAS behave differently from other non-polar organic microcontaminants. Some PFAS have been identified in environmental media in urbanised areas with and without production sites nearby. For example, perfluorooctane sulfonate (PFOS) has been detected globally in a wide array of organisms as well as in non-exposed and exposed human populations. In general, PFAS acute and chronic ecotoxicity to aquatic organisms is moderate to low. Acute toxicity to rodents is also low. While no human health effects or increased cancer risk have been observed for PFAS, PFOS has been shown to effect development and reproduction while perfluorooctanoic acid (PFOA) has been found to be weakly carcinogenic in repeated-dose rat studies. This review will show the importance of filling in the current environmental fate and effects information gaps for PFAS. As such, areas for future research will be suggested.

Environmental fate studies of fluorotelomer intermediates, fluorosurfactants, and fluoropolymers.

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Fluorotelomer intermediates are used to manufacture fluorosurfactants and fluoropolymers, which provide unique properties in a wide variety of consumer products. Fluorotelomer intermediates were selected for study because they were expected to be among the possible compounds into which the fluorosurfactant and fluoropolymer products may potentially degrade. Our environmental fate research has focused primarily on the fluorotelomer intermediate 8-2

Telomer B Alcohol [8-2 TBA; $CF_3(CF_2)_7CH_2CH_2OH$], which we have shown to be hydrolytically stable ($t_{½}$ > one year) and non-toxic to microorganisms at concentrations greater than 100 mg 8-2 TBA L^{-1}. Results indicate, however, that the 8-2 TBA can undergoes transformations in the presence of adapted cultures of microorganisms. The 8-2 TBA appears to partition primarily to the solid and air phases but not to water. Our research in this area has now expanded to include environmental fate studies on the fluorotelomer-based fluorosurfactants and fluoropolymers. We will summarize the environmental fate studies conducted by DuPont on the 8-2 TBA, including an air/water/soil partitioning experiment. We will also discuss recent hydrolytic stability and biotransformation studies performed on the fluorotelomer-based fluorosurfactants and fluoropolymers.

Analytical challenges in determination of Telomer 8-2 Alcohol and Telomer-derived fluorosurfactants and polymers in biological and environmental matrices.

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Environmental fate studies of fluorotelomer intermediates used to produce surfactants and polymers.

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ABSTRACT- Fluorotelomer intermediates, such as the Telomer B 8-2 Alcohol [$CF_3(CF_2)_7CH_2CH_2OH$], are used to manufacture surfactants and polymers, which provide unique properties in a wide variety of consumer products. Fluorotelomer intermediates were selected for study because they are thought to be among the compounds into which the surfactant and polymer products may potentially degrade. Measured water-solubility and vapor pressure of this and three other purified and well-characterized intermediates [$CF_3(CF_2)_nCH_2CH_2X$, where n = 5 or 7 and X = OH or I] are from about 50 times to more than 600 times different from values estimated by a commonly available environmental fate model. Furthermore, these compounds have been shown to adsorb strongly onto surfaces and, as such, require rigorous method development for sampling, measurement, and recovery. The Telomer B 8-2 Alcohol is not toxic to aerobic microorganisms at concentrations of at least 10 mg L^{-1} (measured water solubility is about 140 g L^{-1}). This presentation will summarize environmental fate studies conducted by DuPont, including partitioning and hydrolysis studies. The results of metabolism studies of the Telomer 8-2 Alcohol using activated sludge as the microbial inocculum will be reported. We will also discuss the steps being taking to directly study the environmental fate of fluorotelomer-based surfactants and polymers.