BizNGO 2014

Sponsored by: TOXSERVICES Toxicology Risk Assessment Consulting

December 8th Poster Presentations

5pm at the reception!

1. A Case Study in the Application of Two Chemical Hazard Assessment Frameworks: GreenScreen for Safer Chemicals and the Plastics Scorecard by Mikaela DeRousseau et al.
2. Economic Impact Assessment of Alternative Products based on Life Cycle Analysis by Xiaonan Wang et al.
3. Framework for Automated Hazard Assessment by Kristopher Wehage et al.
4. Greener Solutions: Safer Alternatives to Product Preservation by Heather Buckley et al.
5. Greener Solutions: Eliminating Methylene Diphenyl Diisocyanate (MDI) from Spray Polyurethane Foam Insulation: Alternatives and Assessments by Jeremy Faludi et al.
6. Nitrogen Heterocycles as a Hydrogen Alternative in Polymer Electrolyte Membrane Fuel Cells: an Electrochemical and Toxicological Study by Leah K. Rubin et al.
7. Using Computational Toxicology And Functional Toxicogenomic Approaches To Elucidate Structural Features Of Furan Biofuel Candidate Compounds Contributing to Genotoxicity by David Faulkner et al.

---

1. A Case Study in the Application of Two Chemical Hazard Assessment Frameworks: GreenScreen for Safer Chemicals and the Plastics Scorecard

Authors: Mikaela DeRousseau, Kayla Kuhl, Julie Schoenung
University of California, Davis

Abstract: As public concerns grow about the hazards of chemicals in everyday products, companies are more aware of needing to find alternatives to make products safer. It is common for companies to avoid chemicals on a case-by-case basis when public concern or regulations make one chemical no longer suitable for use in products; however, simply waiting to discover that a chemical is hazardous or toxic should not be preferred. Chemical hazard assessments (CHA) are a better way to ensure that chemicals in a product are safe before manufacturing and public use. This presentation explores the application of two chemical hazard assessment frameworks created by Clean Production Action – the GreenScreen for Safer Chemicals and the Plastics Scorecard. As a case study, we apply both CHA methodologies to the bill of substances for a representative computer hard drive to evaluate the benefits and limitations associated with each framework.

---

2. Economic Impact Assessment of Alternative Products based on Life Cycle Analysis

Authors: Xiaonan Wang and Julie M. Schoenung
Department of Chemical Engineering and Materials Science
University of California, Davis

Abstract: Economic impact is an important factor to consider during the implementation of Safer Consumer Products (SCP) regulations, particularly in the process of Alternatives Analysis (AA). To build up an environmentally and economically sustainable future, it is of significance to focus not only on material and energy flows, but also on the external impacts such as the environmental and economic impacts. This work includes a review of state-of-art Economic Impact Assessment (EIA) methods, a proposed framework to incorporate EIA into AA in conjunction with Life Cycle Assessment (LCA), and actual case studies to demonstrate the methodology. A primary case study is conducted to evaluate the life-cycle economic impacts of alternative options for desktop computer displays by integrating the economic impact indicators into process simulation tools and obtaining the quantified values for comparison simultaneously with the process design, including materials handling and recycling.

---

3. Framework for Automated Hazard Assessment

Authors: Kristopher Wehage, Panan Chenhansa, Julie M. Schoenung
University of California, Davis

Abstract: *GreenScreen for Safer Chemicals* is a framework for comparative chemical hazard assessment and is the first transparent, open and publicly accessible framework of its kind, allowing manufacturers and governmental agencies to make informed decisions about the chemicals and substances used in consumer products and buildings. In a GreenScreen assessment, an overall chemical hazard rating is assigned for each chemical or substance based on eighteen hazard end-points from up to thirty different sources. The result is a simple numerical benchmark score that allows GreenScreen practitioners to flag chemicals of concern and identify safer alternatives. Although the benchmarking procedure is straightforward, aggregating and sorting hazard data is tedious, time consuming and prone to human operator error. In light of these challenges, the present work demonstrates how much of the data collection and benchmarking procedure can be automated. The steps involved in automated assessment include 1.) culling chemical hazard data from the world wide web, 2.) assigning hazard meta-data, 3.) translating from native database representation to GreenScreen representation using the the GreenScreen "List Translator" and 4.) carrying out the GreenScreen benchmarking process. The procedure is carried out by a computer program written in the Python programming language, and generates GreenScreen benchmark scores and detailed hazard data for over 1400 chemicals in less than a minute. Discussion of the potential benefits and limitations of automated techniques is provided. By embedding the program into a web-based graphical user interface, the extensibility of the Python code is demonstrated. The website interface also demonstrates how automated hazard assessments can coexist with and augment manual assessments. Source code is provided and made freely available to the hazard assessment community.

Greener Solutions: Safer Alternatives to Product Preservation

Authors: Heather Buckley, Adam Byrne, Billy Hart-Cooper, and Jiawen Liao
University of California, Berkeley Center for Green Chemistry

Abstract: Antimicrobials are an essential component of all water-based home and personal care products. By preventing the growth of bacteria, moulds, and fungi, they extend the shelf life of these products and protect consumers from unpleasant or dangerous exposures. However, many antimicrobials in current commercial products are non-selective, and their impacts on human health and the environment can have unintended consequences ranging from acute sensitization to chronic health effects such as neurotoxicity. In this work, we take a biomimetic approach to designing safer preservative systems. Based on literature and patent review

and in partnership with Biomimicry 3.8, Seventh Generation, and Beautycounter, we recommend alternative strategies to be tested within the design constraints of home and personal care products.

Greener Solutions: Eliminating Methylene Diphenyl Diisocyanate (MDI) from Spray Polyurethane Foam Insulation: Alternatives and Assessments

Authors: Jeremy Faludi, Patrick Gorman, Tina Hoang
University of California, Berkeley

Abstract: California Department of Toxic Substances Control (DTSC) has identified methylene diphenyl diisocyanate (MDI) as a Chemical of Concern in spray polyurethane foam (SPF) applications. SPF is commercially valuable and widespread because of its high insulation value, its long lifetime, and its ability to be sprayed onto surfaces or into cavities in buildings. MDI is a key component of SPF because its strong cross-linking imparts SPF with short curing time (easy foaming) and longevity (chemical and physical stability). However, MDI has been recognized as an occupational asthmagen via respiratory sensitization. This project's goals were therefore to 1) Identify alternative materials and/or processes to meet SPF's performance specifications while reducing hazards and 2) Recommend frameworks for evaluating alternatives in terms of both function and health hazard. Our research suggested protein-based cross-linkers, foamed concrete, and non-isocyanate polyurethane (NIPU) present the most viable alternatives to MDI-based polyurethane and warrant further development. Three other alternatives were considered worthy of further research in the long term, and three additional alternatives were considered unpromising. For the evaluation framework, we developed a table that tracks 14 physical/chemical properties and 11 hazard criteria. These attributes were selected to track crucial functional properties, human health hazards, and ecotoxicity of SPF replacements. The list of alternatives and the evaluation framework should help future researchers, industry, and regulators evaluate materials for MDI substitution in SPF applications.

Nitrogen Heterocycles as a Hydrogen Alternative in Polymer Electrolyte Membrane Fuel Cells: an Electrochemical and Toxicological Study

Authors: Leah K. Rubin, Elise Deunf, Kyle T. Clark, Sébastien Gottis, David Faulkner, Chris D. Vulpe, John B. Kerr, John Arnold
University of California, Berkeley

Abstract: One of the challenges facing widespread adoption of hydrogen-powered fuel cells is the fuel itself, since hydrogen is difficult to obtain, store, and transport. Various hydrogen storage systems have been proposed, including "virtual hydrogen storage": a hydrogenated liquid organic compound that can be electrochemically dehydrogenated in a fuel cell to produce protons and electrons directly. Nitrogen heterocycles have been shown to have favorable thermodynamics for thermally reversible hydrogen storage, and could be good candidates for fuels in a virtual hydrogen storage system. Two potential fuels, indoline and *N*-ethyldodecahydrocarbazole, have been studied through a variety of electrochemical techniques. We have shown that appropriate redox mediators and bases can be used to tune the fuel oxidation potential and promote formation of the dehydrogenated product. We are also exploring the broader implications of nitrogen heterocycles as fuels with a toxicity study.

Using Computational Toxicology And Functional Toxicogenomic Approaches To Elucidate Structural Features Of Furan Biofuel Candidate Compounds Contributing to Genotoxicity

Authors: David Faulkner, Breanna Ford, Chris Hill, John Hartwig, Marty Mulvihill, Dale Johnson, Mike Fasullo, Chris Vulpe

Abstract: Furan compounds, specifically, 2,5-dimethylfuran (2,5-DMF) have been the subject of intense interest as biofuels in recent years, as they have a similar energy density to gasoline, yet can be renewably derived from carbohydrates. Furans have additional appeal as biofeedstocks, potentially replacing petroleum-based feedstocks for chemical synthesis. Problematically, previous work suggests that furan-containing compounds may be chemically reactive, leading to adduct formation - raising concerns about the safety of furans as biofuel candidates or chemical feedstocks. For example, recent work by Fromowitz et al. indicates that 2,5-DMF has clastogenic and genotoxic effects in murine hematopoetic cells. However, our understanding of the structural features of furans and furan derivatives which influence genotoxicity remains incomplete. We are therefore carrying out a systematic analysis of the chemical features which mediate the genotoxicity of furans. A collaboration with organic chemists has produced several candidate compounds with discrete changes in the functionalization and saturation of the furan ring. We hypothesized that these subtle changes may affect the reactivity and thus, genotoxicity. Initially, we used a computational approach to assess the furan compounds for predicted genotoxicity endpoints and found that these approaches were limited in their ability to differentiate between simple furans and furan derivatives. We used functional toxicogenomic profiling as well as selected DNA-repair mutants to explore the relative genotoxicity of the compounds. Our preliminary results indicate that the location of small R groups on the furan rings and the degree of ring saturation substantially influence toxicity of the furan compounds.