ABSTRACT

BizNGO-Chemical Footprint Conference
December 8 & 9, 2015 • JFK Library, Boston, MA

Greener Approach to Material Sciences

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Human curiosity is the source of all the inventions that have made our lives very comfortable. The risk we have taken in this regard is the price we have paid for this progress. Humans have taken the risk of using new materials without completely understanding the problems associated with them. The starting materials for most of the organic chemicals used today are petroleum based and most often the products are not environmentally degradable.

Biological systems reveal functionality that often exceeds man-made products. Biobased materials can also serve as a renewable hydrocarbon source that can help fashion the next generation of advanced functional materials. This approach is illustrated in two examples where biobased feedstock is used for the synthesis of functional alternative to toxic materials.

First, the synthesis of novel bio-novolac phenolic resins using naturally occurring carbonyl containing sugars or sugar derivatives as a substitute for formaldehyde will be presented. These novel biobased novolac can be cured with conventional curing agents such as hexamethylenetetramine. Preliminary studies indicate that this new class of bio-based phenolic resins exhibit promising properties and have the potential to be used as an alternative to phenol-formaldehyde.

Biobased and bio-inspired surfactants are the second class of materials that will be discussed. Non-ionic surfactants such as octylphenol ethoxylates (OPE), are classified as a substance of very high concern (by the European Union regulation, because it degrades into toxic octyl phenols. These chemicals are being phased out as they are harmful to aquatic life and have endocrine disrupting effects. Here we report the synthesis of a novel sugar based surfactant with both hydrophilic and hydrophobic segments using benign reaction conditions. The surface tension of hydrophobically modified sugar is similar to that of the OPEs. The Hydrophilic-Lipophilic Balance (HLB) of this sugar-based surfactant can further be tuned by attaching polyethylene glycol chains. The possibility of conversion of bioderived sugars into sustainable and safe alternative surfactants has been demonstrated.

The benefits for the pursuit of materials research using biobased feedstock and green chemistry transcends sustainability considerations and often opens exciting possibilities from a scientific and commercial perspective.

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Hansen Solubility Parameters in Practice (HSPiP) Software

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Solvents with toxic properties are used for numerous applications: adhesives, spot removers, paint thinners, dry cleaning, nail polish removers, etc. The Toxics Use Reduction Institute (TURI) in partnership with UMass Lowell faculty and students are utilizing the Hansen Solubility Parameters in Practice (HSPiP) Software to identify safer solvent and solvent blends to provide safer alternatives to the use of toxic solvents. TURI currently has two projects underway: 1) finding safer solvents to replace toluene, acetone, and hexane in contact adhesives, and 2) finding safer solvents to replace methylene chloride in paint stripping products.

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Identifying Safer Chemicals using Hansen Solubility Parameters

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Contact adhesives are composed of polymers dissolved in solvents and are used to adhesively bond materials together. This class of adhesives works by being applied to the surfaces that are to be bonded and, once the solvent evaporates, the two materials are brought into intimate contact thereby forming a strong bond. Toluene, hexane, and acetone are commonly used to solvate polychloroprene and SBR rubbers that are used in contact adhesives. These organic solvents are considered toxic under the Massachusetts Toxic Use Reduction Act (TURA) and have demonstrable acute and long-term health effects on humans, animals and the environment. Long-term exposure to toluene has been shown to permanently damage the brain causing loss of speech, hearing, muscle control and memory. Long-term inhalation exposure to hexane may lead to neuropathy, while long-term exposure to acetone can lead to headaches, dizziness or unsteadiness, which can be dangerous in a factory or lab setting. Here, we describe a process to identify safer alternatives to toluene, hexane, and acetone using the software program *Hansen Solubility Parameters in Practice* (HSPiP). The poster will also review the testing and screening of potential alternative solvents. Once identified, these alternate solvents will be tested for solubility, evaporation rate, ease of application and bond strength.

Polyester resins that are commonly used in the open mold manufacturing of composites contain styrene monomer, which is volatile and is a carcinogen, respiratory irritant, skin irritant and reproductive toxin. In order to reduce the exposure of workers to styrene vapors, alternative monomers were identified using Hansen Solubility Parameters. These monomers were tested in polymerization and trimethylolpropane diallyl ether was able to reduce the styrene content by 50%.

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"Greener" sample preparation of lycopene from tomato (Lycopersicon esculentum) for extraction and quanitification by UV/Vis spectrophotometry and high performance liquid chromatography

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Lycopene is the major carotenoid found in red-fleshed fruits, and is known to have antioxidant properties that are important to human health. Traditional methods employed in sample preparation to determine lycopene content include the initial extraction of the carotenoid from fruit tissue, followed by a partitioning step to remove water and polar carotenoids from the sample. This type of method relies on the use and disposal of hazardous organic solvents, such as tetrahydrofuran (THF) and petroleum ether. An analytical method to determine lycopene content in tomato using 'greener' solvents and lower solvent volumes with respect to those used in traditional extraction methods was developed. During the initial extraction of lycopene, 2-methyltetrahydrofuran (2-MeTHF) was used as an alternative to THF, as it has fewer known health hazards and is more sustainably produced than THF. During extraction in preparation for determination of total carotenoid content in tomato using spectrophotometric analysis, traditional and green solvents were compared using UV-vis spectrophotometry. Preliminary results suggest that the use of 2-MeTHF produced comparable results comparable to THF. Heptane and ethyl acetate were studied as replacements for petroleum ether, the solvent typically used for the partitioning step in preparation for HPLC analysis used to determine the carotenoid profile in tomato. When the 'green' solvents were compared to petroleum ether in the partitioning step, preliminary data suggests that these solvents were not comparable to petroleum ether. However, it may be possible to reduce the volumes of petroleum ether may be successfully employed, reducing the environmental hazards associated with this step.

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Environmental, Health and Safety Data Resources

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TURI has developed a comprehensive Subject Guide, entitled, *Environmental, Health and Safety Data Resources*, to facilitate research on chemical hazards. This Guide provides links to various governmental and research databases, as well as authoritative lists that can be used to identify hazards associated with chemicals of concern. TURI's Research and Reference Specialist will be available to answer questions about the Guide and other resources available at the TURI Library for chemical hazard research.