

Research Highlights

2013 Chemical Safety Research Accomplishments

EPA's Chemical Safety for Sustainability Research Program (CSS) is designed to conduct innovative research and generate impactful science to help inform decisions made about chemical safety. In 2013, EPA's chemical safety researchers:

- [Developed methods to accelerate the pace of chemical screening](#)
- [Protected vulnerable species and groups such as children](#)
- [Fostered solutions for sustainable materials](#)
- [Developed computational models to understand the relationship between chemical exposures and human health outcomes](#)
- [Evaluated the potential effects of chemicals of interest](#)

Accelerating the pace of chemical screening

Screening Data on Thousands of Chemicals

EPA completed Phase II of the multi-year [Toxicity Forecaster](#) (ToxCast) project, and on December 17, 2013, publically released [new high-throughput screening data](#) on 1,800 chemicals evaluated in over 700 high-throughput screening assays. This data is available on the ToxCast webpage and through the interactive [Chemical Safety for Sustainability](#) (iCSS) dashboard.

In order to address challenges with data translation, accessibility, and usage, the EPA is hosting several stakeholder outreach activities such as workshops and webinars to ask for stakeholder feedback. The first stakeholder workshop was held on January 14, 2014 in Research Triangle Park, NC. The second ToxCast stakeholder meeting will be held April 2-3, in Washington, DC followed by a ToxCast Phase II data summit in May. More information about registering for the stakeholder workshops and other upcoming events can be found [here](#).

High-Throughput Exposure Predictions & Curating Exposure Data

EPA researchers developed high-throughput exposure models to predict exposures for 1,763 chemicals using production volume, environmental fate and transport models, and a simple indicator of consumer product use. The models are being improved by adding more refined indoor and consumer use information. The Chemical and Product Categories database (CPCat) catalogs the use of over 40,000 chemicals and their presence in different consumer products. The chemical use information is compiled from multiple sources while product information is gathered from publicly available Material Safety Data Sheets (MSDS). EPA researchers are evaluating the possibility of expanding the database with additional product and use information. This database is explained in more detail in a published paper located [here](#).

NexGen

Phenomenal advances in molecular systems biology, improved understanding of gene-environment interactions, reports from the National Research Council, and volumes of new toxicity data from the United States and Europe are rapidly changing the landscape of chemical risk assessment. In



September, 2013 EPA researchers released the draft report [Next Generation Risk Assessment: Incorporation of Recent Advances in Molecular, Computational, and Systems Biology](#) for public review and comment. The draft report describes the multiyear NexGen program which aimed to develop and evaluate new risk assessment approaches that take full advantage of molecular, computational, and systems biology research and methods. Beginning in 2014, EPA will enter the next phase of this effort in which novel data streams generated by ToxCast and related research will be used to enhance and accelerate EPA's risk-based chemical evaluations

Protecting vulnerable species and groups

[Markov chain nest productivity model \(MCnest\)](#)

EPA scientists have linked pesticide application and toxicity data to information ecologists use to evaluate the life history and reproductive success of bird species, creating an accessible, easy to use model that can be applied to each pesticide application scenario under consideration. This model, the [Markov Chain Nest Productivity Model](#)



(MCnest), has recently been improved by EPA scientists and can be used by EPA and its stakeholders to predict the extent of ecological impact of pesticides. The success of this effort demonstrates how complex data from a variety of sources can be integrated to improve the quality, effectiveness, and efficiency of EPA decisions.

Fostering solutions for sustainable materials

[Product Category Rules \(PCR\)](#)

Recently, EPA co-led an international initiative with 30+ organizations in 11 countries to develop guidelines to help purchasers across the federal government select the most environmentally-friendly and safe products. The challenge with coming up with such guidelines is that there are different standards for communicating environment performance on labels, making comparison of environmental performance information on labels very difficult. To address this difficulty, [EPA announced draft guidelines](#) on [Product Category Rules \(PCR\)](#), that provide product category specific requirements and guidelines for calculating and reporting environmental impacts across the full life cycle of a product using life cycle assessment (LCA).

Ultimately PCRs will allow comparable analyses of products' environmental impacts. PCR is a voluntary, international effort with more than 40 participating organizations dedicated to improving this ongoing guidance document. The European Union has recently launched a [Product Environmental Footprint](#) program that will use this guidance to develop the rules for labels for European products. There has recently been an increase in demand for standardized environmental information for building products

in the US, in part because of the new [LEED 4.0 green building standards](#) making credits available for products with these labels.



High-Throughput Tools for Nanomaterials Fate and Transport

Because quantifying the mobility of engineered nanoparticles (ENMs) in hydrologic pathways from point of release to human or ecological receptors is essential for assessing environmental exposures, EPA researchers are developing a high throughput screening technique for nanoparticle transport using 96 deep well plate columns packed with porous media.

This method is being evaluated to address the traditional time-consuming and labor-intensive methods of measuring ENMs transport and fate in the environment. Current results showed that this screening technique produced highly reproducible column hydrodynamic properties and retention levels consistent with the existing literature. This technique obviates the need to run repetitive tracer tests and is well suited for rapidly screening the mobility of ENMs in porous media.

More information about this new technique is described in a paper available [here](#).

Developing computational models

Virtual Embryo

EPA is working on the [Virtual Embryo Project](#) (v-Embryo)—aimed at developing new methods that use high-tech computer modeling and vast collections of data and biological knowledge-bases in place of traditional lab tests. These models are intended to assess the different ways that exposure to chemicals in the environment during pregnancy might disrupt the development of an embryo. Using a selection of everyday chemicals with known health effects in animals, researchers are working to build computer-based virtual models of embryo development. A [paper](#) about the blood vessel development model was published April 4, 2013 in “PLoS Computational Biology.”

Evaluating potential effects of chemicals of interest

Perfluorinated Chemicals Paper Published in *Environmental Science & Technology*

In order to test for potential perfluoroalkyl acids (PFAAs) uptake and bioaccumulation into crops grown in bio-solids-amended soils, EPA’s Region 5 office, EPA Office of Research and Development, the Colorado School of Mines (CMS), and the Metropolitan Water Reclamation District of Greater Chicago tested various crops in both field and controlled greenhouse environments.

The results demonstrated that PFAA uptake can occur in edible compartments of most crops grown in biosolids-amended soil. However, uptake is dependent upon several different factors: plant type, PFAA concentrations, soil properties, and analyte. Additionally, across all studies, the findings show preferential uptake of carboxylates over sulfonates, and accumulation of shorter chain PFAAs over longer chain PFAAs. Further information about this project can be found [here](#)

Dr. Steven Thomas Purucker Receives PECASE Award

On December 23rd, [President Obama named NERL's Dr. Steven Thomas Purucker](#) one of 102 recipients of the annual Presidential Early Career Awards for Scientists and Engineers (PECASE). This is the highest honor bestowed by the United States Government on science and engineering professionals in the early stages of their independent research careers. Winners can receive up to a five-year grant to pursue their research. Dr. Purucker works in EPA's Office of Research and Development in the Ecosystems Research Division of the Exposure Research Lab.

Dr. Elaine Hubal on advisory committee for Health Canada's Chemical Management Plan

CSS's Deputy National Program Director, Dr. Elaine Cohen Hubal, has been appointed by Environment Canada and Health Canada to serve on their Chemicals Management Plan (CMP) Science Committee. The committee functions as an external advisory body to the Canadian government, providing scientific expertise to support the strong science foundation required for the Chemicals Management Plan (CMP). As a member of the committee, Dr. Hubal will help advise on issues associated with evaluating the potential impacts of chemical substances used in commercial and industrial products on public and environmental health.

Will Boyes joins the Neurotoxicology and Teratology Journal Editorial Board

Dr. William K. Boyes, Interim Associate National Program Director of Chemical Safety and Sustainability (CSS) at the EPA, is a new member of the editorial board for the *Neurotoxicology and Teratology Journal*. *Neurotoxicology and Teratology* is a provider of science and health information, dedicated to publishing new information regarding the effects of chemical and physical agents on the nervous system. Boyes's research at EPA focuses on the use of engineered nanoparticles (ENPs) in consumer products and their potential effects on humans and the environment

Event Announcements

REGISTER TODAY: ToxCast Stakeholder Workshop & Data Summit

To solicit stakeholder feedback on the new Toxicity Forecaster (ToxCast) chemical screening data, the EPA is hosting a stakeholder workshop in Washington D.C. on April 2-3, 2014 and a Data Summit in Research Triangle Park, NC on May 13-14, 2014. On January 13, EPA held the first ToxCast stakeholder workshop to provide an overview of the recently released ToxCast high-throughput data from screening thousands of chemicals and demonstrated the online Chemical Safety for Sustainability dashboards. Registration and information about the Stakeholder Workshops and Data Summit is available [here](#).

CSS @ ACS Green Chemistry Conference

CSS National Program Director (NPD) Dr. Tina Bahadori is co-chairing the American Chemical Society's 18th Annual Green Chemistry and Engineering Conference: Advancing Chemistry, Innovating for Sustainability on June 17 through June 19, 2014. Deputy NPD Dr. Elaine Cohen Hubal will also be co-

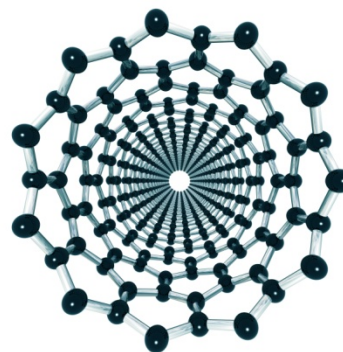
chairing the “Chemical Design: Minimizing Adverse Impact and Assessing Alternatives” theme. For more information, visit the conference website [here](#).

Computational Toxicology Communities of Practice Presentation

On February 27, EPA’s Computational Toxicology Communities of Practice will feature a presentation to give a presentation about the increased chemical space covered by ToxCast and new chemical structure files. More information about Computational Toxicology Communities of Practice, past presentations, or how to become involved is available [here](#).

May 2014 Nanomaterials Meeting

The UC Center for Environmental Implications of Nanotechnology (UC CEIN) will host an invitational meeting for *Categorization Strategies for Engineered Nanomaterials in a Regulatory Context*. The focus of this meeting will be to discuss recent advancements in the field of nanotechnology research and ongoing research. For more information visit the center website [here](#). Information about current EPA nanomaterials research is available [here](#).



Mark Your Calendars: 2014 Society of Toxicology Annual Meeting

Remember to register for the Society of Toxicology Annual meeting March 23-27, 2014 in Phoenix, AZ. EPA researchers will be instructing select Continuing Education Classes such as *Systems Pathway-Knowledge Tools for Constructing AOPs* with Daniel L. Villeneuve and *Benchmark Dose Modeling* by Qiyu (Jay) Zhao. The conference includes scientific presentation and poster sessions where many EPA scientists will be presenting their latest chemical safety research. Visit the [conference website](#) for detailed information about registration, housing and more.

A Successful Future of Toxicology Meeting

FutureTox II, a Contemporary Concepts in Toxicology meeting held by the Society of Toxicology in Chapel Hill, NC, highlighted several fascinating presentations by EPA researchers. Those researchers include Keith Houck, Richard Judson, Daniel Villeneuve, and SOT Co-Chair and conference moderator Thomas Knudsen. The conference was dedicated to investigating the central question: *In what ways can in vitro/in silico methodologies be seen as superior to in vivo methods such that the latter would not be needed to confirm findings?* Visit the [meeting website](#) for presentation slides and program information.

Funding & Employment Opportunities

EPA Awards Developmental Neurotoxicology Adverse Outcome Pathway Grants

EPA announced over \$3 million in grants to research institutions to fund studies to map how chemicals interact with biological processes and how these interactions may lead to altered brain development. Awardees include: North Carolina State University, Raleigh, NC; The University of Georgia, Athens, GA; University of California, Davis, CA; and Sanford-Burnham Medical Research Institute, La Jolla, CA. These grants focus on developing better adverse outcome pathways (AOPs), models that predict the connection between exposures and the chain of events that lead to an unwanted health effect. Meet the grantees and learn about their research plans at the Kickoff Meeting held at the Society of Toxicology annual meeting in Phoenix, AZ. For more information, please see the [press release](#).

EPA Research Funding Available

Organotypic Culture Models

EPA is requesting research proposals for Organotypic Culture Models (OCM) for Predictive Toxicology. The selected proposals will receive funding to accelerate research in predictive toxicology through the formation of research centers focused on the development and evaluation of OCMs. This request was released on September 23rd and will remain open until January 23rd, 2014. Interested applicants can find more information [here](#).

Ecological Exposure Models

EPA is requesting research proposals for the development of systems-based models to evaluate the ecological impacts of manufactured chemicals. The selected proposals will receive funding for their research. This request for proposals will close on March 4, 2014. Interested applicants can find more information [here](#).

EPA is Accepting Applications for ORISE Postdoctoral Positions

As part of the Oak Ridge Institute for Science and Education (ORISE) Internship/Research Positions Program, EPA is accepting applications for [postdoctoral positions](#). Some positions for chemical safety research are listed below.

- [Sustainable Synthesis and Applications of Nanomaterials and Nanocomposites](#)
- [Application of Computational Chemistry to Predictive Toxicity Modeling](#)
- [Chemical Safety for Sustainability](#)
- [Human Behavioral Exposure](#)
- [Applying Novel Data Streams to Advance Human Health Risk Assessment](#)

Chemical Safety Research in the News

[Chemical Engineering News Features Article about EPA's Predictive Toxicology Research](#)

[US EPA Releases Data from High-Throughput Screening](#)

[EPA Consumer Product Database May Help EPA Select Chemicals](#)

Visit EPA's Chemical Safety Web Page Regularly for Updates

www.epa.gov/research/chemicalscience