

U.S. EPA's Office of Research and Development

Center for Computational Toxicology and Exposure **Russell Thomas, Director**

- I. What are your Center's key current scientific capabilities?
- 2. How can the scientific capabilities in your Center be used to address future environmental problems, and what challenges or barriers exist for your Center to do so?

Provided for the NASEM committee on Anticipatory Research for EPA's Research and Development Enterprise to Inform Future Environmental Protection The views expressed are those of the author and do not necessarily reflect the views or policies of the US EPA

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CCTE Key Scientific Capabilities

Chemical Characterization

- Library of environmental and industrial chemicals and reference compounds
- QSAR modeling and systematic read across

• Hazard Evaluation

- Human health and ecological high-throughput assay development and testing
- Organotypic model development
- Fish, amphibian, invertebrate, and rodent in vivo testing
- Computational modeling of cell, tissue, and organ-level responses
- Cross-species extrapolation
- Adverse outcome pathways

Toxicokinetics

- Human and ecological toxicokinetic assays (in vitro and in vivo)
- Traditional TK, PBPK, and HTTK modeling and in vitro-to-in vivo extrapolation
- Environmental persistence and bioaccumulation of methodologically challenging chemicals

• Exposure Assessment

- High-throughput, multi-pathway human and ecological exposure models
- Non-targeted analysis
- Traditional analytical chemistry quantification in water, sediment and biological tissues

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CCTE Key Scientific Capabilities

Freshwater Coastal Ecology

- Traditional large water sampling (Lake Explorer) with remote/autonomous sensing capabilities
- Computational modeling of freshwater ecosystem dynamics

Ecosystem Services

- Integrated research approaches linking contaminated site characterization with restoration of environment, community-driven productive use, and revitalization outcomes
- Health Impact Assessments projecting health and well-being outcomes from multiple remedial and restoration scenarios of contaminated sites

• Scientific Computing, Data Curation, and Data Management

- Development of integrated data visualization and decision support software tools
- Data curation, management, and mining
- Curated databases of chemistry, physical-chemical properties, ecological hazard, human hazard, chemical functional use, human biomonitoring, ecological monitoring

Outreach and Training

Application of Scientific Capabilities to Future Environmental Challenges

Application of Scientific Capabilities

- Reduce the time required to thoroughly test chemicals and other emerging materials for human health and ecological toxicity from years to months.
- Expand our understanding of quantitative human and ecological exposures for thousands of chemical substances and emerging materials.
- Reduce the time required to characterize freshwater ecosystems and project the future state of ecological condition and ecosystem services from decades to years.
- Develop a comprehensive information system that contains relevant actionable chemical safety and ecological data with the software tools to integrate them for a range of human health and environmental decisions.

Challenges or Barriers

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- Lack of nimble and timely research support infrastructure
- Aging workforce and loss of scientific personnel to retirement
- Growing and sustaining a culture of innovation where it is safe to fail
- Process overload



Thank you!

