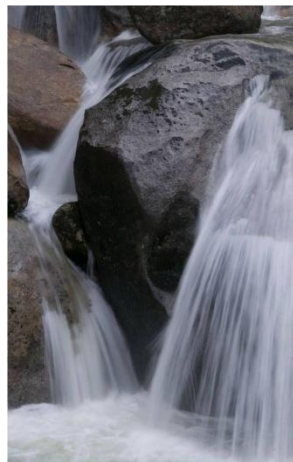


Overview of EPA CSS Intramural Research on Life Cycle and Human Exposure Modeling (LC-HEM)



Kent Thomas and Jane Bare
New Methods in 21st Century Exposure Science Grantees Meeting
February 3, 2015

Project Team Members

Project Leads	National Risk Management Research Laboratory	National Exposure Research Laboratory
<p>Kent Thomas (NERL)</p> <p>Jane Bare (NRMRL)</p>	<p>David Meyer Wes Ingwersen Ray Smith Michael Gonzalez Gerardo Ruiz-Mercado Paul Randall Mark Mason Paul Harten Susan Csiszar (ORISE)</p>	<p>Dan Vallero Jianping Xue Peter Egeghy Cecelia Tan Shi Liu Marsha Morgan Carry Croghan Kathie Dionisio Jingtao Lu (ORISE) Santosh Ghimire (ORISE)</p>
<p>Key Matrix Interfaces</p>	<p>Douglas Young</p>	<p>John Kenneke</p>

Sustainability Research Drivers

U.S. EPA Sustainability Research Strategy 2007

Long-Term Chemical and Biological Impacts

Improving our use of materials, shifting to environmentally preferable materials, and protecting human health all rely on assessing and eliminating the long-term impacts posed by harmful chemical and biological materials.

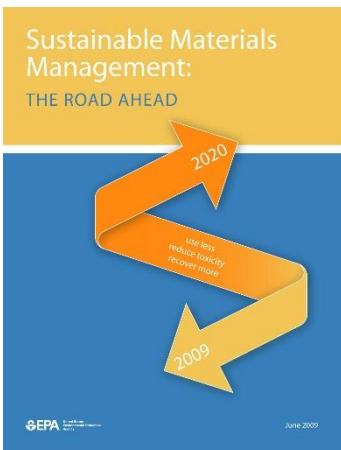
NRC Report: Sustainability and the EPA (the Green Book) 2011

How can the EPA decision-making process rooted in the environmental risk assessment/risk management paradigm be integrated into this new sustainability framework?

Science Challenge



Look for the label!



California Department of
Toxic Substances Control



LC-HEM Science & Tools for Programs, Regions, States

Information and tools are needed for more rapid evaluation of chemical exposure and safety across the life cycles of chemicals and products to support

- Chemical screening/prioritization
- Chemical decision-making
- Alternatives assessments
- Sustainable materials management
- Improved indoor air quality; building components, green building systems
- Green chemistry initiatives

Research Objectives

Develop a framework and database structure that brings together life cycle and chemical exposure modeling for more rapid assessments

Implement high priority/high interest case studies for demonstration and evaluation of the framework and tool

Construct a user-friendly tool for evaluating chemical/product impacts in a life cycle assessment framework to support decision-making through improved risk and sustainability analysis

Anticipated Impact

Impact Summary

The proposed research will improve evaluation of chemical risk in a life cycle assessment framework to support Agency decision-making to enhance safety and promote sustainability.

Success Will Include

Improved human exposure modeling in life cycle assessments

Modeling and assessment for chemicals/products with less extensive data

More rapid and higher throughput assessments

LC-HEM tool usable by Offices/Regions

Adoption and use inside/outside Agency

Research Approach – LC-HEM Tasks

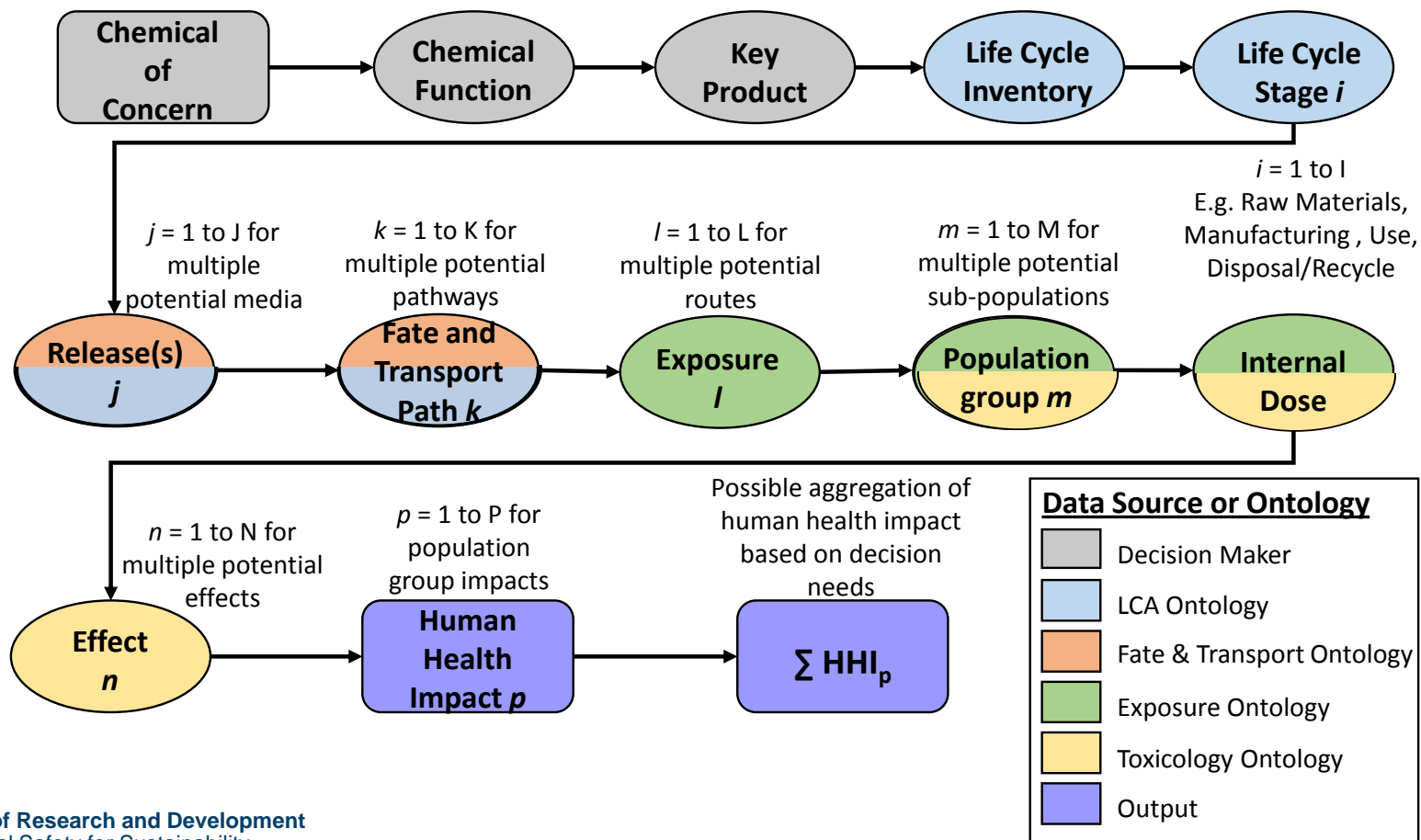
Task 1 – LC-HEM Conceptual Framework Development	FY15	Product	Jane Bare Dan Vallero
Task 2 – Initial Case Study for Demonstration and Evaluation	FY15 – FY16	Key Product	Kent Thomas Dave Meyer
Task 3 – Resource Description Framework Development	FY15 – FY17	Key Product	Wes Ingwersen
Task 4 – HEM Life Cycle Development & Evaluation	FY15 – FY17	Product	Dan Vallero
Task 5 – Rapid Estimation of Life Cycle Inventory	FY15 – FY17	Product	Ray Smith
Task 6 – Development of Beta LC-HEM Tool	FY16 – FY18	Key Product	TBD
Task 7 – Case Studies for Demonstration and Evaluation	FY17 – FY19	Products	TBD

Research Approach – LC-HEM Tasks

Task 8 – Spray foam insulation methods and characterization	FY15 – FY16	Product	Mark Mason
Task 9 – Solvent substitution software tool (PARIS version III)	FY15 – FY15	Product	Paul Harten
Task 10 – LC-HEM Tool	FY18 – FY19	Key Product?	TBD

Task 1 – Conceptual Framework

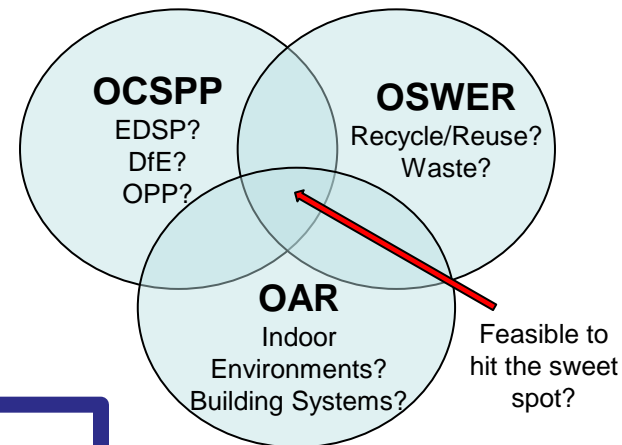
Complete and publish a framework that brings together chemical exposure and life cycle modeling for supporting environmental decision-making through improved risk and sustainability analysis



Task 2 – Case Study for Demonstration/Evaluation

Select, implement, and publish a case study

- Exercise framework across multiple life cycle stages
- Data rich product/chemical to support evaluation
- Demonstrate relevance for Partners



Considerations for the Initial Case Study Selection

Program Relevancy

- Demonstrate Relevance for Partner(s)
- Active CSS Research in Other Projects

Chemical/Product Selection Examples

- Flame Retardants – building or consumer products
- EDC – consumer products
- Pyrethroid Insecticide – consumer products

Case Study Selection

LCA Considerations

- Well defined LC stages
- Secondary data for LCI construction (emissions, products, processes) and spatial distribution

HEM Considerations

- Chemical appears in multiple LC stages
- Known exposure pathways and dose information
- Available data for modeling and evaluation

Prioritization

- Product
 - Interior use building material or furnishing material
 - Material goes into recycling and waste
 - Production process data availability
- Chemical
 - SVOC
 - Potential EDC, possibly on TSCA workplan list
 - Exposure data availability, preferably on NHANES list

Task 2 – Case Study for Demonstration/Evaluation

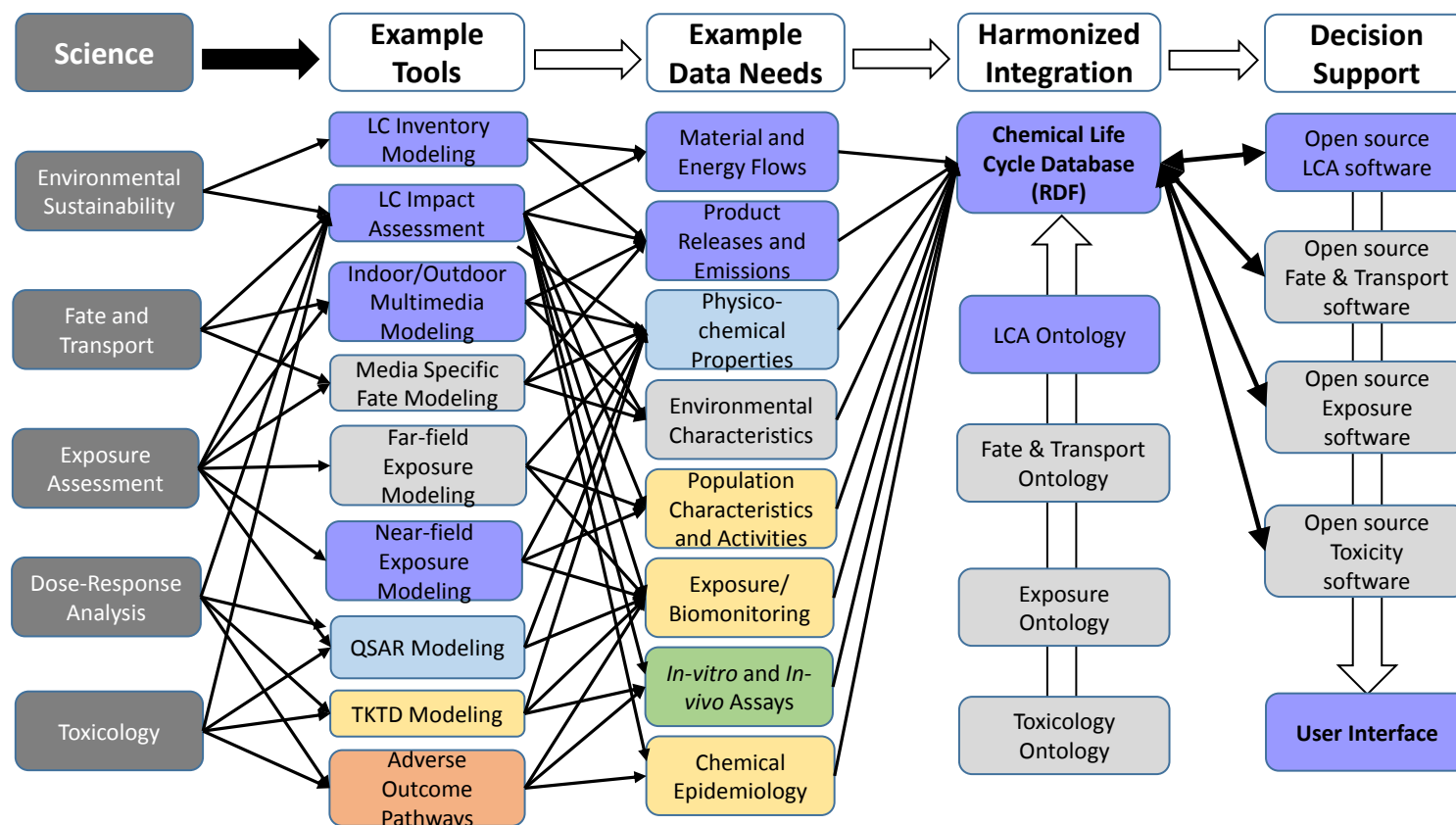
Example Selection

- Polyurethane foam used in furniture/mattresses
- Recycled/reused as carpet padding; recycled/reused in other plastics; used as a combustion fuel; landfill disposal
- Possible chemicals:
 - High Data: pentaBDEs
 - Likely EDC, not TSCA workplan, no longer used but still present; DfE alternatives assessment
 - Residential occurrence data, exposure data, NHANES
 - Low Data: TCEP (Tris(2-chloroethyl) phosphate)
 - 2014 TSCA workplan addition; EDC??; part of DfE alternatives assessment
 - Uncertainty in extent of use in PUF
 - No/limited exposure data, not in NHANES

Task 3 – Resource Description Framework

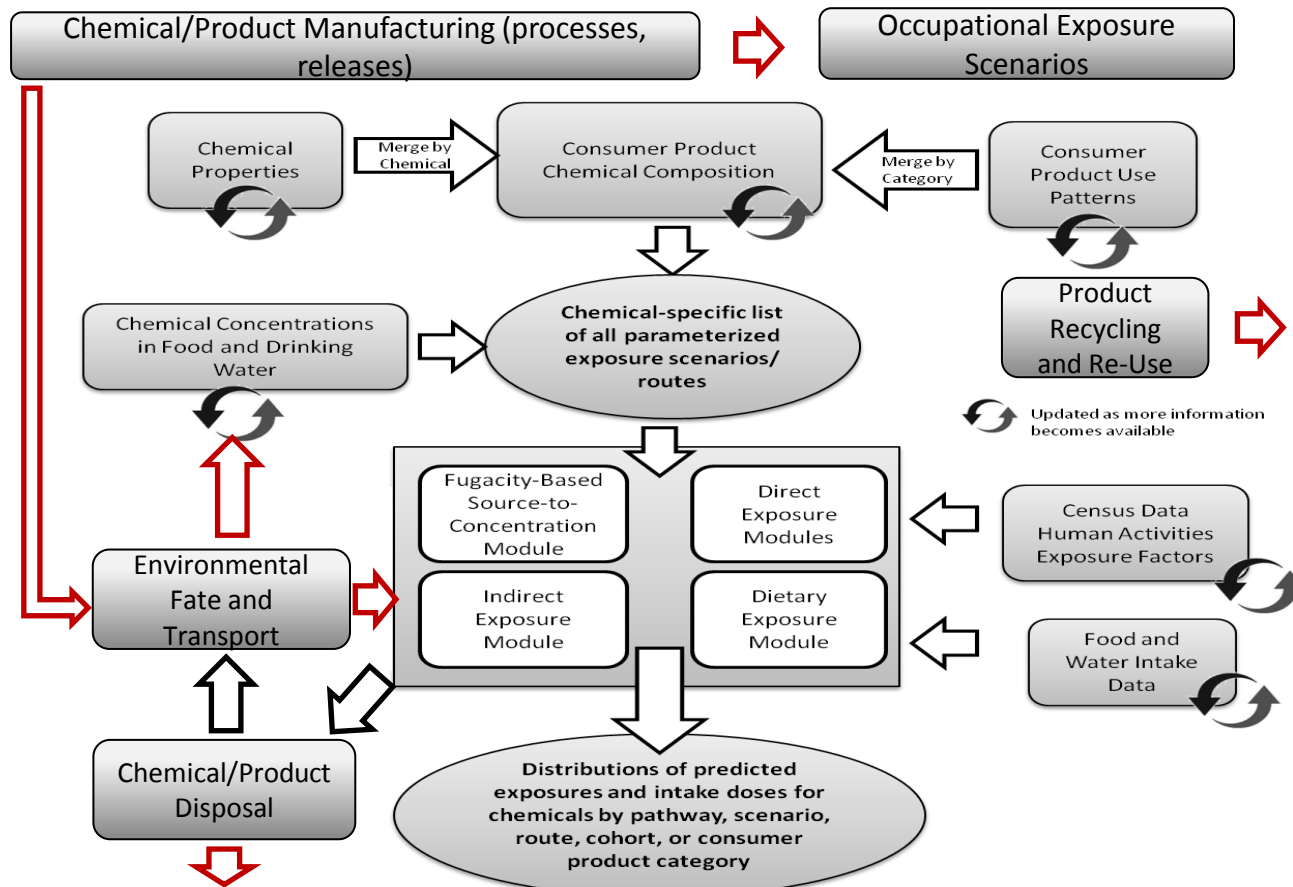
Develop RDF for harmonizing Life Cycle Assessment (LCA), human exposure data, and other data

- Develop and/or integrate relevant ontologies
- Identify key database information sources
- Develop harmonization software tool



Human exposure model development across a range of LC stages

- Define exposure scenarios, population groups, and time frames
- Develop, apply, and/or modify appropriate models for exposure and dosimetry
- Evaluate models and uncertainty



Task 5 – Rapid Estimation of Life Cycle Inventory

Purpose:

Develop approaches for rapid estimation of life cycle inventory at chemical and product levels through data mining and model simulation

Task Features:

- Life Cycle Inventory development is first step of LC-HH Assessment
- “Rapid Estimation” needed for new product/chemical combinations
- Combine knowledge of processes and emissions at relevant life cycle stages
- Inventory database will grow over time

Three Methods:

- Top-down – Mining available data to maximize LCI (a.k.a. MADMax)
- Bottom-up – Analysis by building components (a.k.a. ABC)
- Classification & Reconciliation of Release Inventory (CMDL Library)

Task 8 – Spray Polyurethane Foam Insulation

Mark Mason, Xiaoyu Liu



Purpose:

Methods and data for characterizing chemical emissions from SPF in support to OPPT and Federal partners

Task Milestones:

- Evaluate chamber and sampling methods for SPF emissions
- Co-chair ASTM symposium and journal publications
- Evaluate scale-up from small chamber to full-scale systems testing
- Generate emission parameters to support modeling

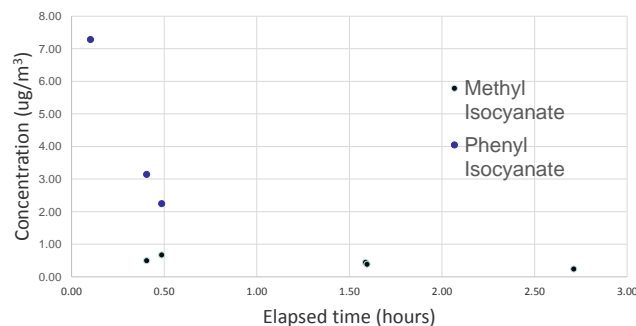
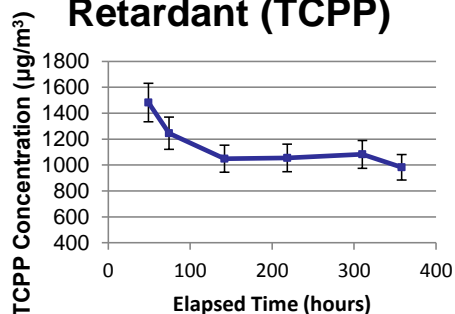
Task Products:

- Consensus (ASTM) methods
- Data to characterize emissions of isocyanates, flame retardants, amine catalysts, propellants, other VOCs

Collaborators:

- Federal: CPSC, NIST, NIOSH, OSHA, CNRC
- Industry: ACC/CPI, Bayer, Air Products
- Consensus testing bodies: ASTM
- Testing Laboratories: IFKAN
- CSS Rapid Exposure SVOC Model Parameters (Liu)

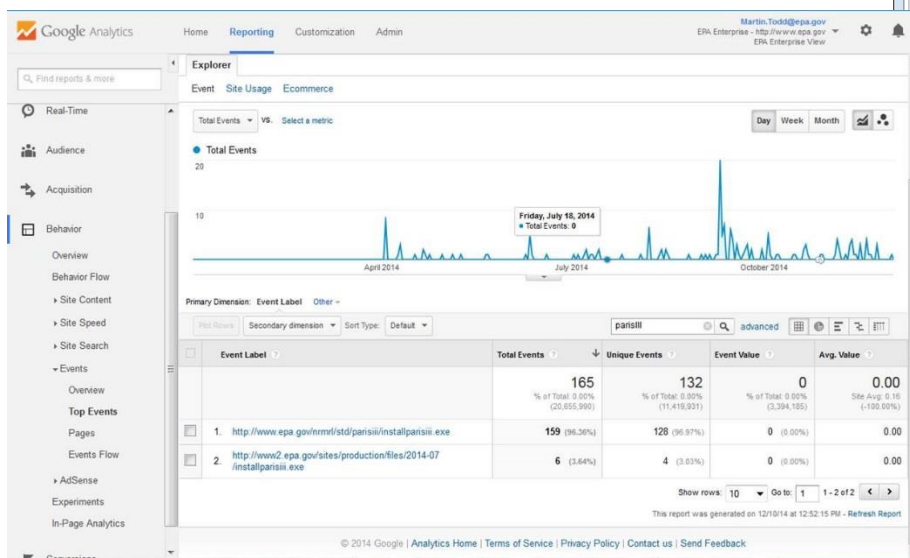
SPF Flame Retardant (TCPP)



Task 9 – PARISIII Solvent Substitution Software Tool

Program for Assisting Replacement of Industrial Solvents (PARIS):

- Used by solvent technicians, chemical and environmental engineers, and environmental consultants to find greener solvents used in industrial processes
- Initial software release FY13; updated PARIS v II release in FY14
- FY15 update to PARIS v III
 - Increase to 5000 solvents
 - Improved miscibility feature
 - Improved ability to identify substitutes



The screenshot shows the PARIS III software interface. The 'Physical Properties' tab is active, displaying a table of properties for a current mixture. The table includes columns for Property, Tolerance(%), Lower, Desired, Upper, Replacement, and Units. A list of replacement solvents is shown on the right, with '3: 1-chloranyl; pentane' selected. The interface also includes a 'Solvent Replacement' table at the bottom right.

Property	Tolerance(%)	Lower	Desired	Upper	Replacement	Units
Molecular Mass	11.0	70.512	79.227	87.942	94.675	kg/kmol
Liquid Density	14.0	8.14E2	9.47E2	1.08E3	8.90E2	kg/m ³
Boiling Temperature	10.0	301.377	334.863	368.349	343.042	K
Vapor Pressure	30.0	1.76E1	2.52E1	3.28E1	2.03E1	kPa
Surface Tension	16.0	1.68E-2	2.00E-2	2.32E-2	2.00E-2	kg/s ²
Viscosity	30.0	3.94E-4	5.63E-4	7.32E-4	6.12E-4	kg/m-s
Thermal Conductivity	30.0	9.10E-2	1.30E-1	1.69E-1	1.20E-1	J/(m-s-K)
Flash Point		281.712			292.708	K
Air Index				8.42E-1	2.50E-1	Impact/Kg
Environmental Index				6.27E0	1.10E0	Impact/Kg
Tolerance Scale Factor						

Solvent	Wt%
1-chloranyl-2-...	80.0
pentane-2,3-diol	20.0

Collaborations & Contracts

OEI/NCC

EMVL support for the beta-version of the LCA Harmonization Tool, Ravi Nair

EPA Program

OAR/IED, Dr. Kelly Scanlon AAAS Science & Technology Policy Fellow

EPA/NSF Networks for Characterizing Chemical Life Cycle (NCCLC) Grantees

University of California at Santa Barbara, Dr. Sangwon Suh

Contracts

University of Michigan, Dr. Olivier Jolliet, Exposure/LC ontologies and case study

TBD - Life cycle ontologies

Potential Areas of Shared Interest

Improved and more rapid indoor models for SVOCs

Data to facilitate parameterization indoor models across a wide range of chemicals (predictive parameterization)

Case studies

Data/information to support case study development and implementation (i.e. flame retardants; spray foam insulation research)

Data to support model and case study evaluation