Consumer products in the home environment: Considerations for indoor air

Kathie Dionisio
U.S. Environmental Protection Agency
Office of Research and Development
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Prepared in collaboration with
Kristin Isaacs and John Wambaugh

What is ORD?

U.S. Environmental Protection Agency

Office of Research and Development (ORD)

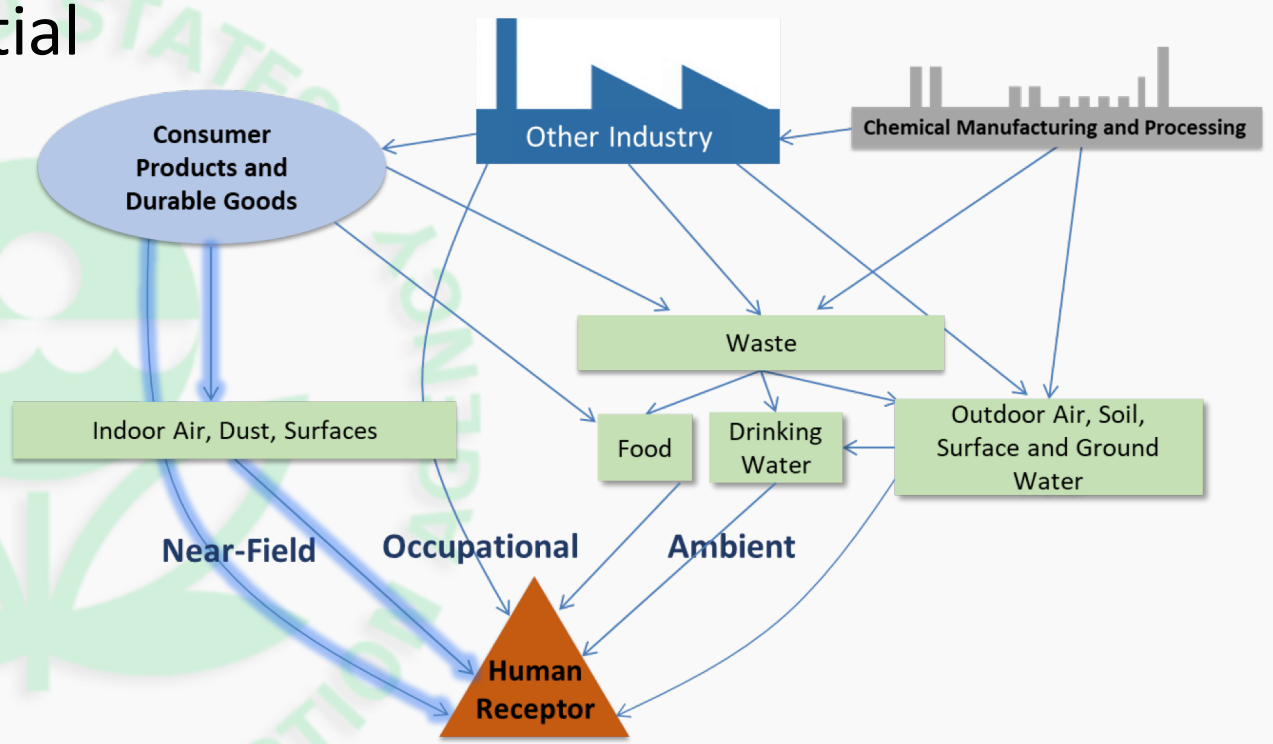
ORD is the scientific research arm of the U.S. EPA, providing the scientific foundation for decisions and actions of the Agency

- Public health and environmental assessment
- Computational toxicology and exposure
- Environmental measurement and modeling
- Environmental solutions and emergency response

Research Triangle Park, NC

Understanding Chemical Exposure Pathways

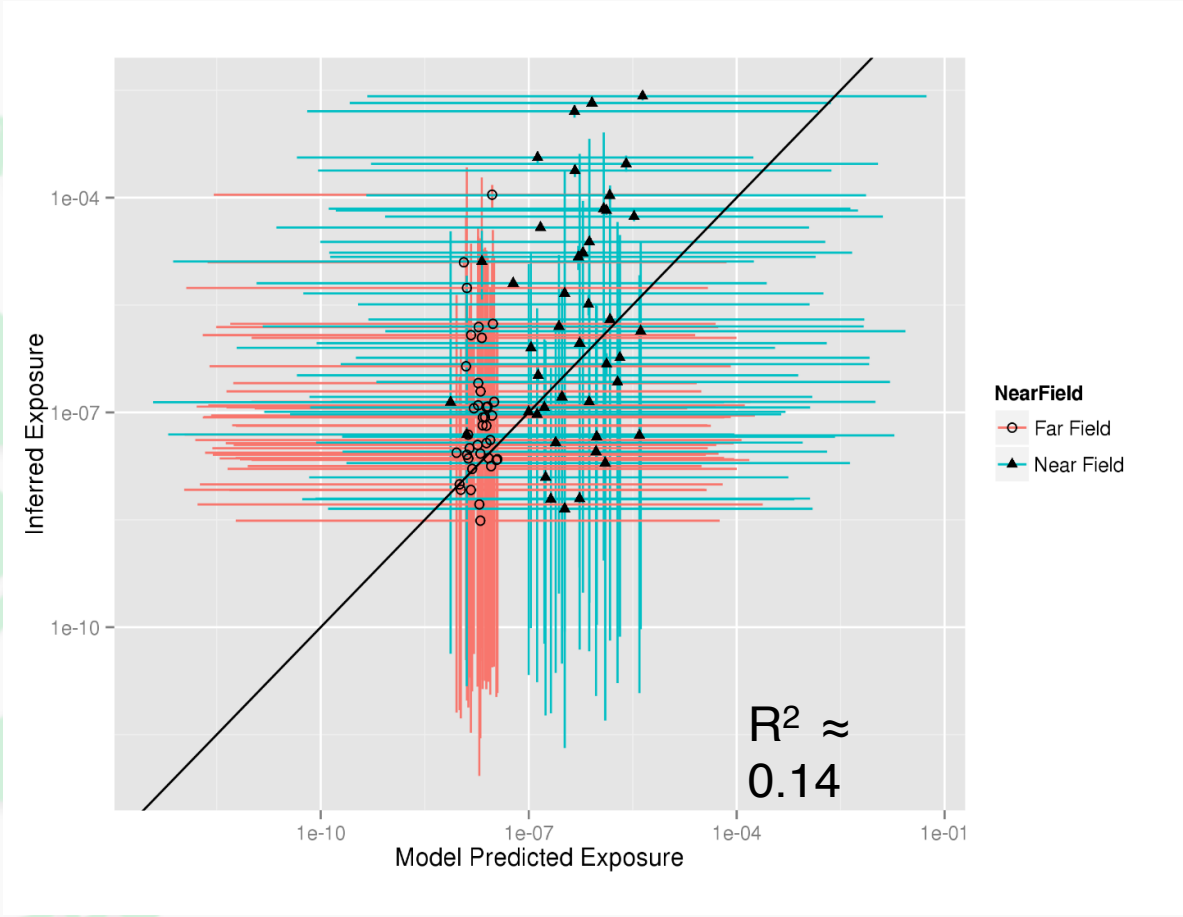
- The U.S. EPA must prioritize thousands of commercial chemicals for further study: which have the highest potential risk?
  - Requires both ***exposure*** and ***hazard*** information
  - Many of these chemicals are data-poor with respect to exposure



There is a need to characterize ***exposure pathways*** for thousands of chemicals

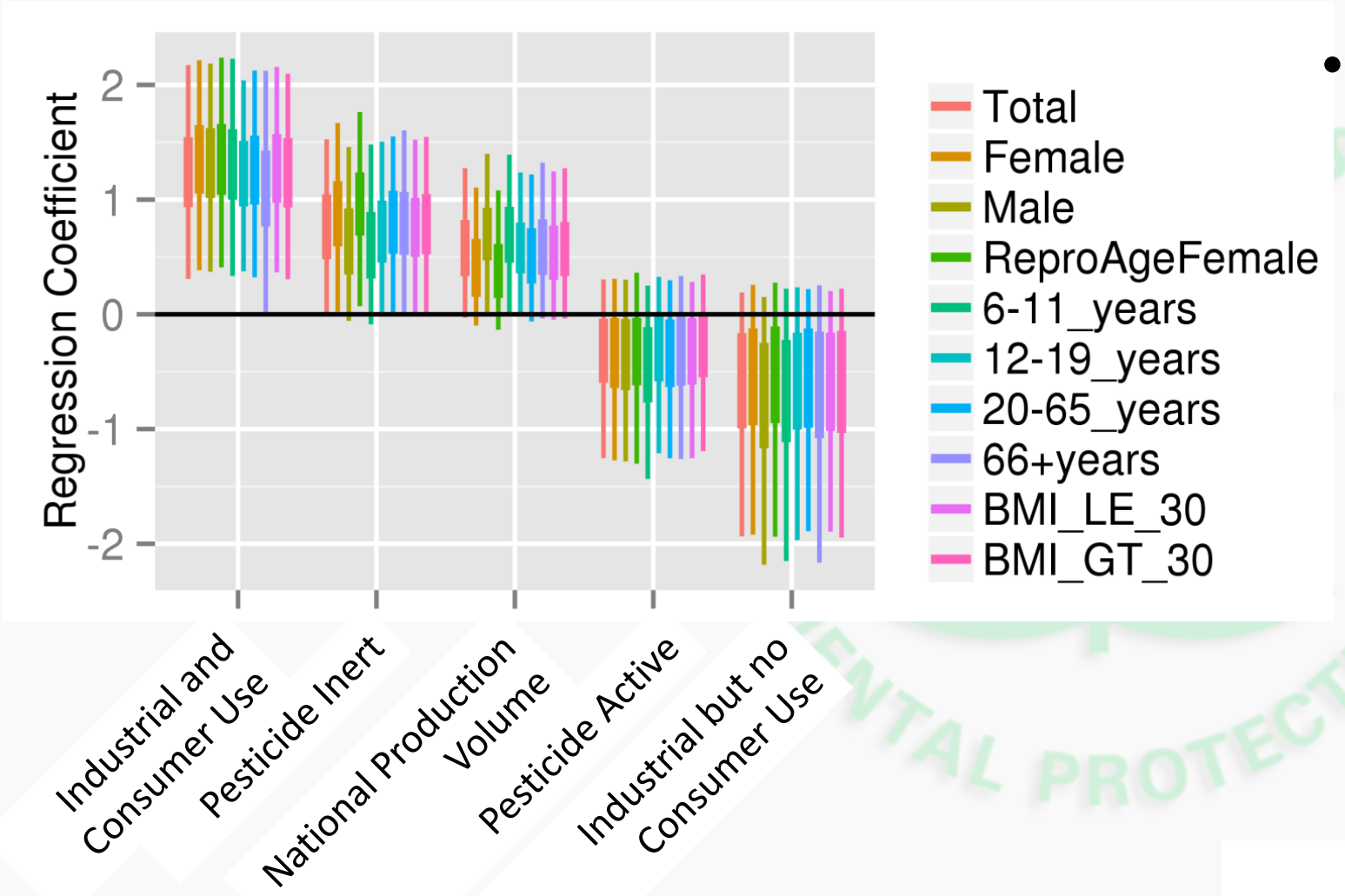
Understanding Chemical Exposure Pathways

Chemicals used in a "near-field" or residential context have higher observed concentrations in biomonitoring studies



Wambaugh et al. 2013

Human exposure is complex



Wambaugh et al. 2014

- We can predict 50% of the chemical to chemical variability in median NHANES exposure rates using 5 predictors
  - Industrial and consumer use
  - Industrial but no consumer use
  - Pesticide inert
  - Pesticide active
  - Production volume

Near-Field Exposure: Critical Questions

- What chemicals are in products (formulations and household articles)?
- Which of these chemicals are released, how, and how much?
- Where do these chemicals reside in the indoor environment (e.g., dust or air)?
- What exposures result (single chemicals, co-exposures?)

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Chemical sources in the home

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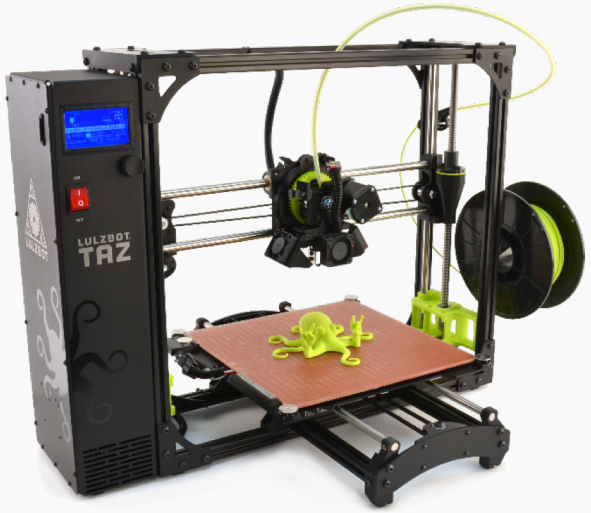
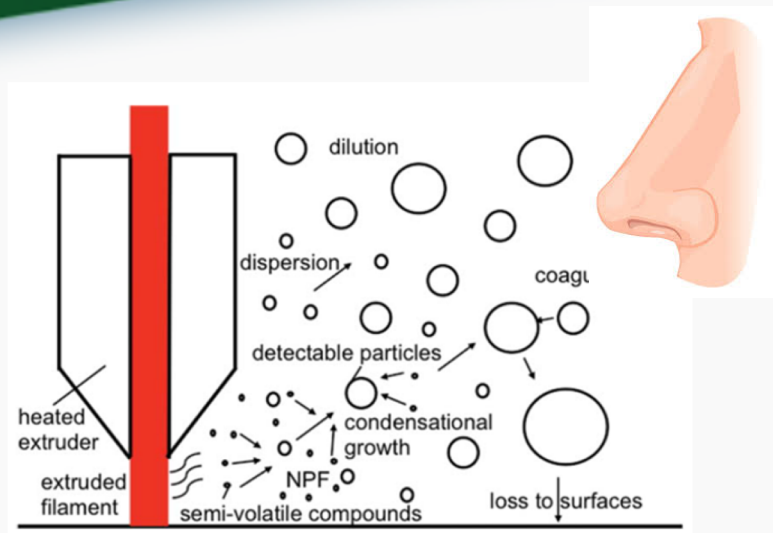
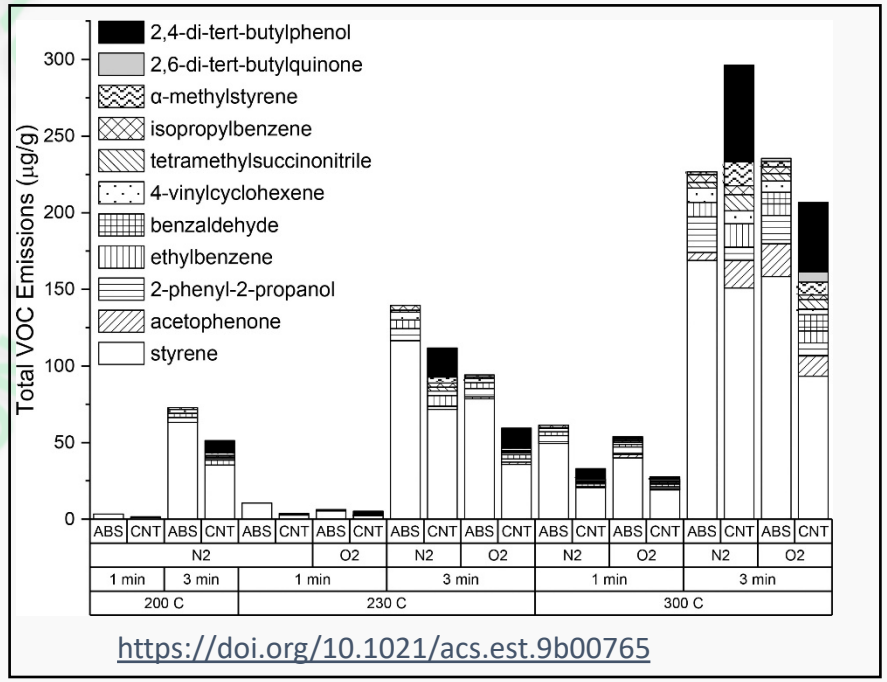
Changing sources



Chemical sources in the home: 3D printers

- Operation of 3D printers produces volatile organic compounds (VOCs) and incidental ultra fine particles (< 100nm) (UFP)
- VOC composition and concentration dependent on polymer type
- UFP form from fragments of the polymer and condensational growth of VOCs
- EPA ORD analysis of filaments, emissions, and human exposure from 3D printing processes
  - Identify physicochemical properties of filaments that correlate with the quantity and composition of incidental nanoparticles and VOCs generated during operation
  - Inhalation exposures can easily go above IRIS reference concentration values during 3D printing processes





https://doi.org/10.1021/acs.est.9b00765

Courtesy Todd Luxton

Chemicals in consumer products

Reported Data

Consumer Product Information Database

- Broad range of consumer products
- Reported chemical content (e.g. from ingredient labels and Safety Data Sheets)

- Reported data on some consumer products, limited composition information
- Dominated by foods

Measured Data

- Testing of consumer products to ensure state and federal rules re. chemical content are met
- 61 reports/studies over 18 years, focused on product type or chemical/chemical class

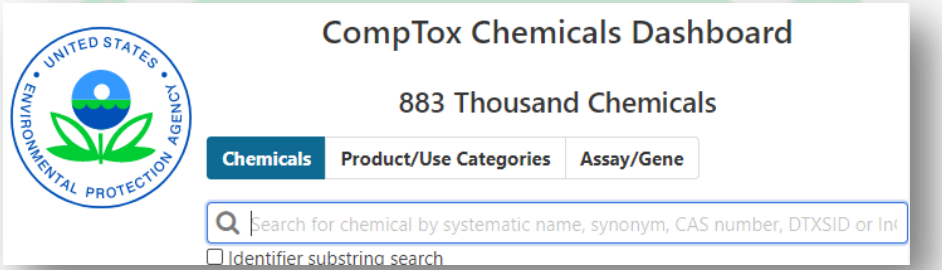
Data needs

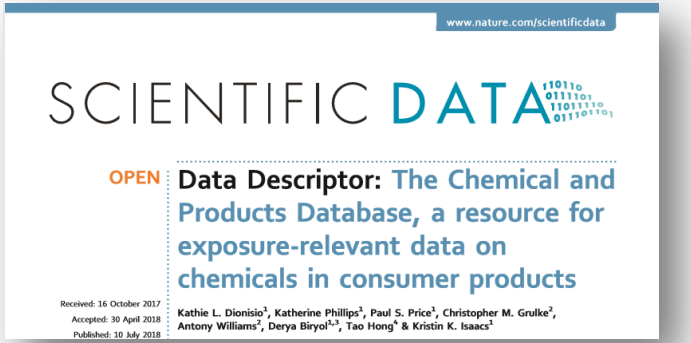
- Harmonization of terms
- Chemical identification
- Tracking of data provenance
- Consistent use of standard product category set
- Consistent process for data updates

Chemicals in consumer products

- Material Safety Data Sheets, ingredient lists, manufacturer disclosures
  - Chemical ingredients in products
  - Weight fraction of chemicals in products
  - Functional use of chemical
- Curated data are released in the **Chemical and Products Database (CPDat)** (Dionisio et al., 2018)

https://comptox.epa.gov/dashboard





https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

Chemicals in consumer products

Arts and crafts/office supplies

Cleaning products and household care

Electronics/small appliances

Home maintenance

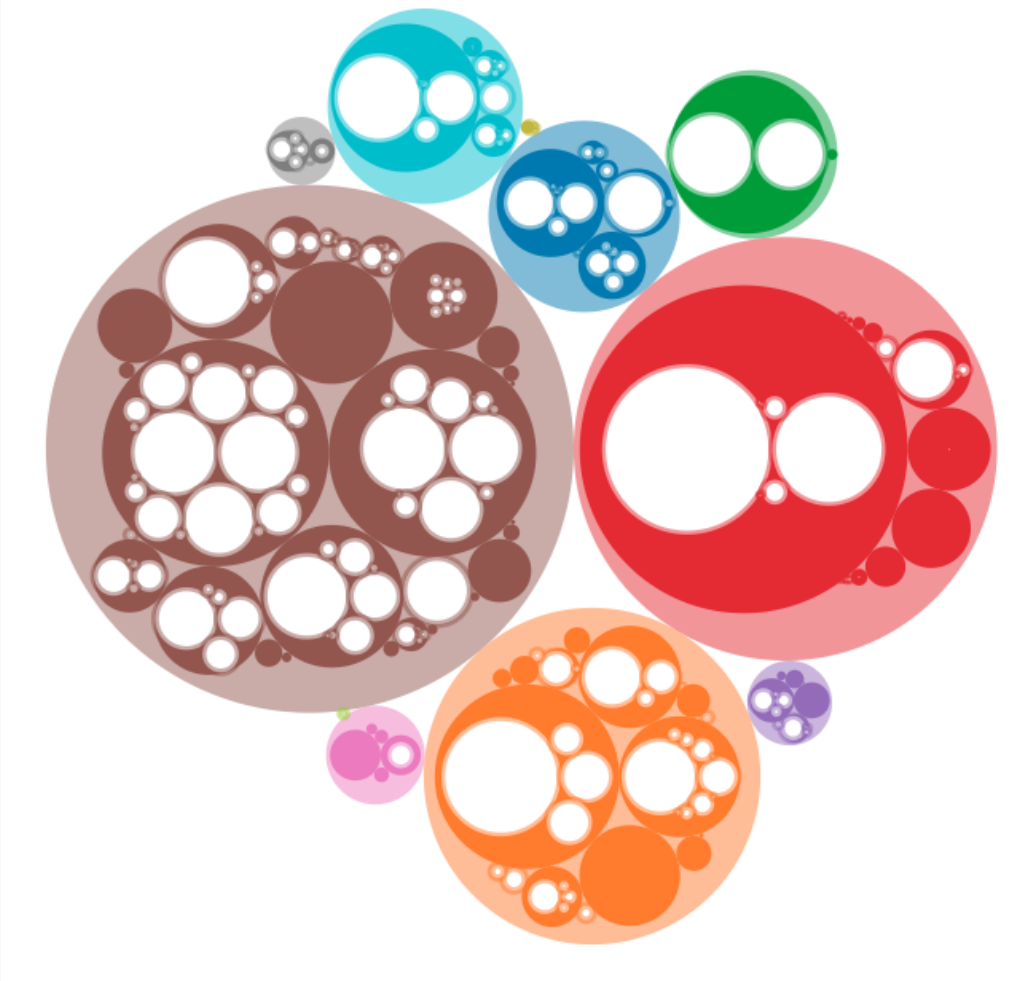
Landscape/yard

Personal care

Pesticides

Pet care

Vehicle



- Includes over **400,000 documents** describing composition of consumer products
- Includes data on **>12,000 unique chemicals** across a wide range of consumer product formulations

CPDat
Chemical and Products Database

Near-Field Exposure: Critical Questions

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- **Which of these chemicals are released, how, and how much?**
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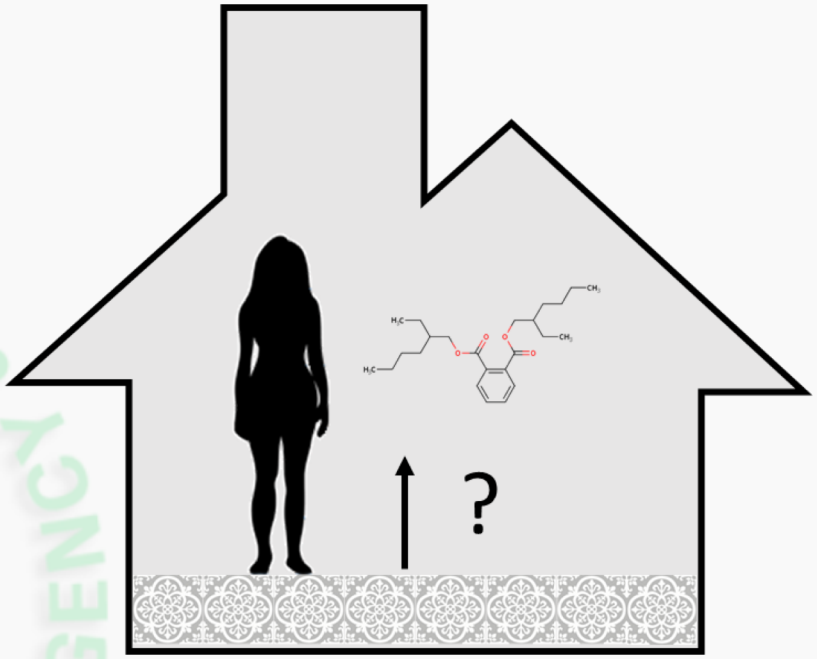
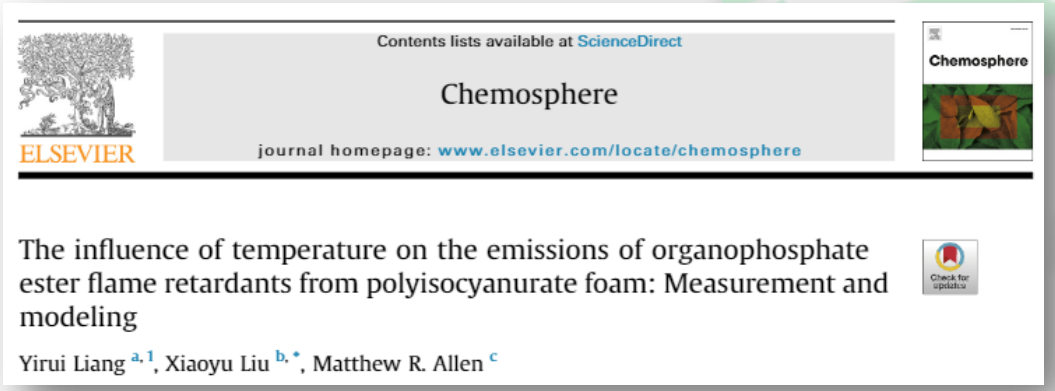
Characterization of emission processes

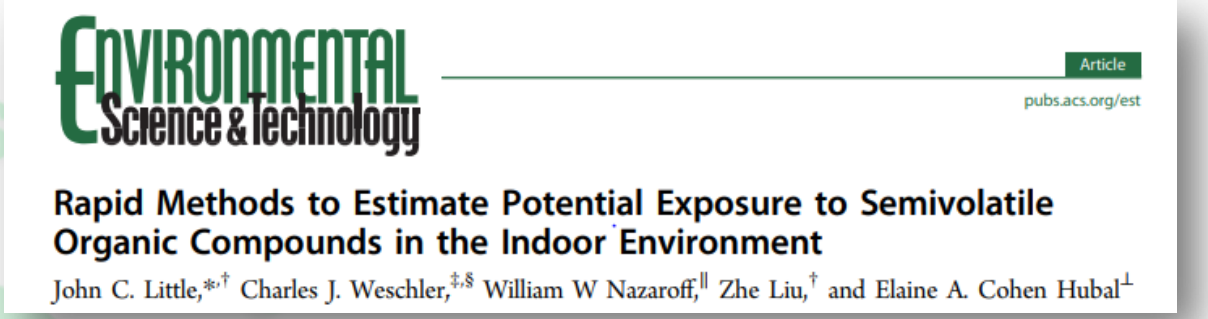
- Many mass-transfer models are available for modeling emission sources for volatile and semivolatile organic compounds (VOCs and SVOCs) in consumer products and building materials such as flooring under different conditions
- Detailed modeling of emission sources depend on parameters such as material/air partition coefficients, solid-phase diffusion coefficients, adsorption/desorption rate constants, mass-transfer coefficients, and initial material phase concentrations (weight fraction in the material)
- Often these parameters can only be estimated using experimental systems (e.g., chamber studies)
- Such work is ongoing in EPA ORD for chemical classes of interest: phthalates, inadvertent polychlorinated biphenyls, organophosphate flame retardants and per- and polyfluoroalkyl substances (PFAS)

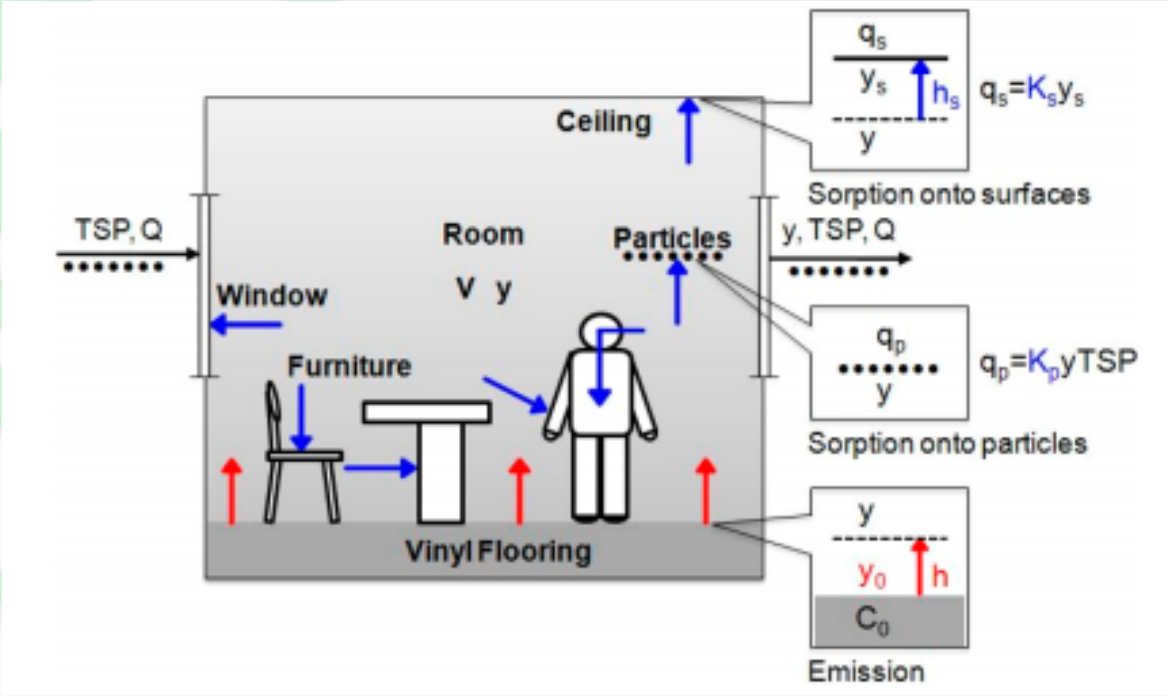




Characterization of emission processes

- For SVOCs with low volatility, emission source models can be simplified in such a way that they depend on a critical parameter, y_0, the steady-state gas phase concentration at the material surface.
- This parameter can be used to parameterize high-throughput exposure models.





Characterization of emission processes

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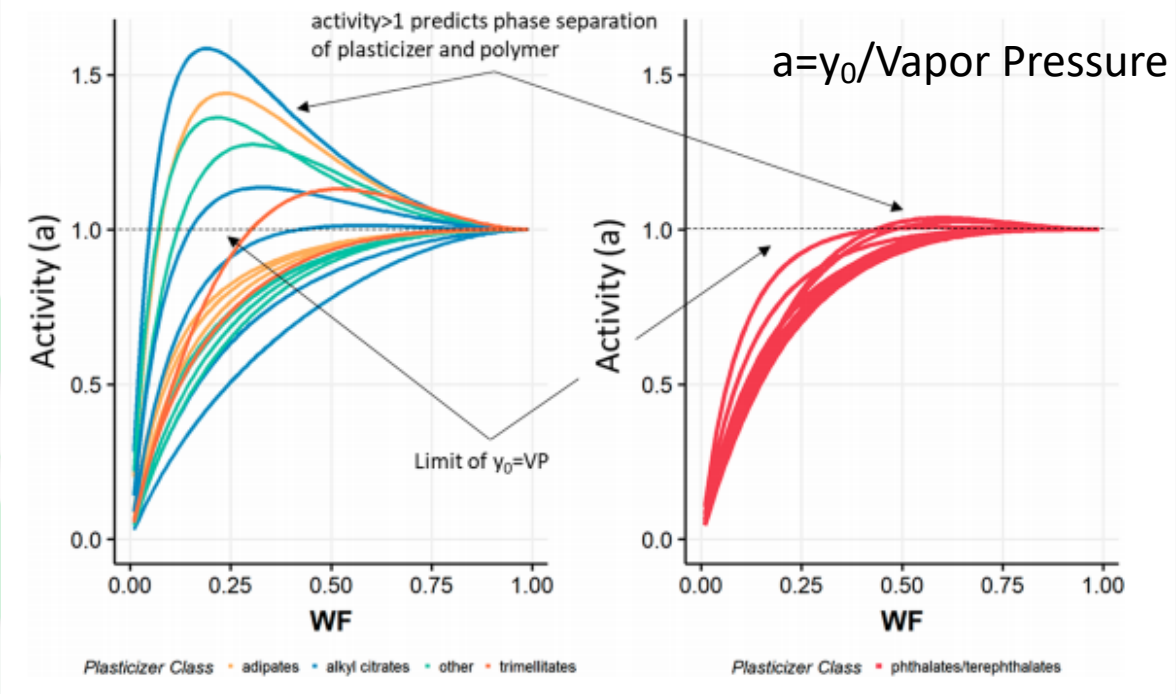
- This parameter can be used to parameterize high-throughput exposure models.
- Structure-based group contribution models can be used to **estimate polymer-chemical interactions** (as quantified by the activity, a: the ratio of the steady state gas phase concentration to vapor pressure) **and y_0** for a variety of plasticizers in PVC as a function of material weight fractions.



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Estimation of the Emission Characteristics of SVOCs from Household Articles Using Group Contribution Methods

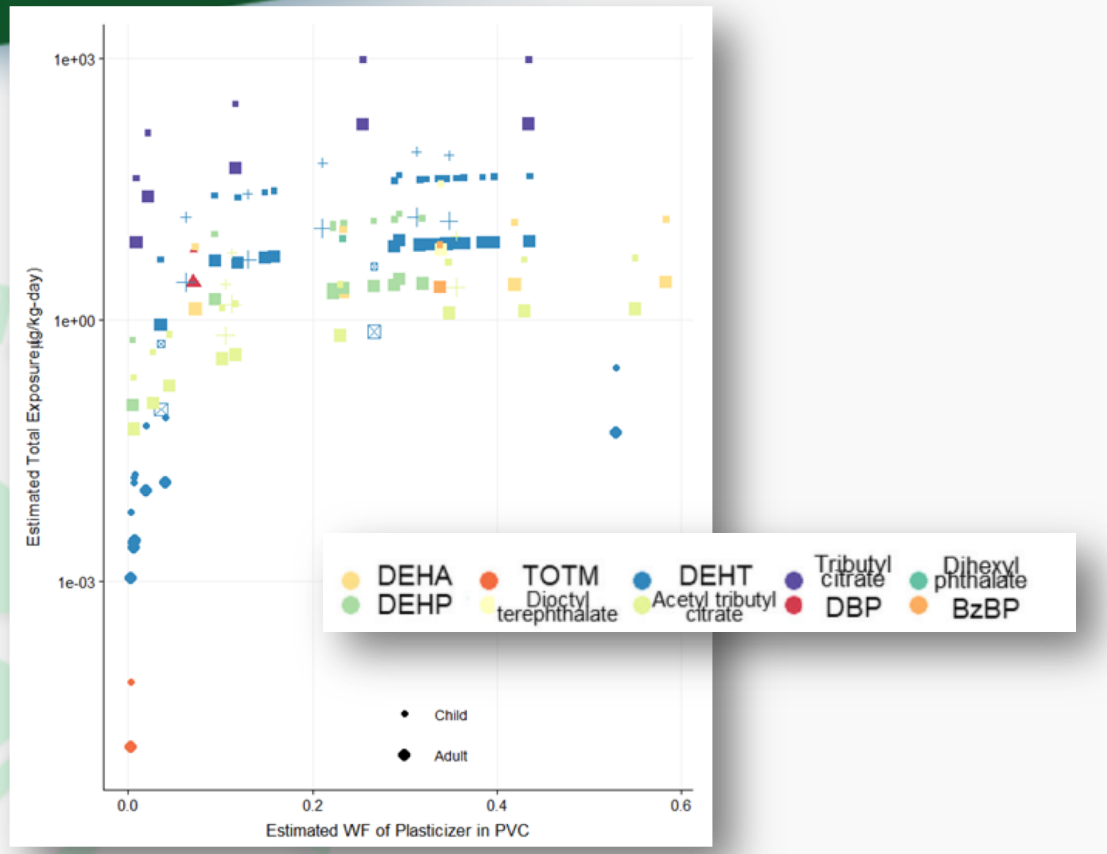
Cody K. Addington,[†,‡] Katherine A. Phillips,[‡] and Kristin K. Isaacs*[,‡]

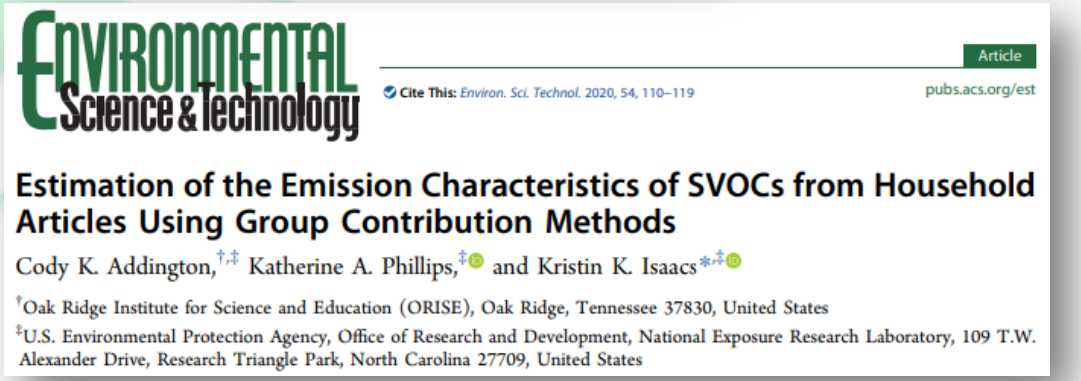
[†]Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, Tennessee 37830, United States
[‡]U.S. Environmental Protection Agency, Office of Research and Development, National Exposure Research Laboratory, 109 T.W. Alexander Drive, Research Triangle Park, North Carolina 27709, United States

Characterization of emission processes

- For SVOCs with low volatility, emission source models can be simplified in such a way that they depend on a critical parameter, y_0, the steady-state gas phase concentration at the material surface.
- This parameter can be used to parameterize high-throughput exposure models.
- We recently applied structure-based group contribution models to **estimate polymer-chemical interactions** (as quantified by the activity, a: the ratio of the steady state gas phase concentration to vapor pressure) **and y_0** for a variety of plasticizers in PVC as a function of material weight fractions.
- This allowed us to estimate high-throughput exposures associated with several different types of products in CPDat.

Allows for estimating high-throughput exposures which were previously limited by gaps in necessary model inputs





Emissions from baby onesies

Chemical detected

Chemical detected

Not detected

Name	1st Dime	2nd Dime	Liquid extract	High temperature emissions	Body temperature emissions
Octacosanol	2152	1.75	14501975		
Octacosanol	2240	1.821	8619612		
n-Hexadecanoi...	1464	1.6	7235571		
Clionasterol	2244	2.912	6058877		
Heptacosane	1936	1.376	5969632	124738	
Octacosane	1988	1.408000	5379752	34850	
Hentriacontane	2136	1.531	5088422		
Triacontane	2088	1.476999	5079738	4809	
Octadecanoic a...	1604	1.568	4910066		
Heneicosane	2020	1.403	4764350		
Nonacosane	2036	1.44	4612815	10035	
Cyclohexane, 1,...	1820	1.349	4487751		
Pentacosane	1826	1.28	4467878	790116	6935
Tetracosane	1906	1.281	4315977	5185	
Tricosane	1706	1.25	4266804	1238940	43127
Hexacosane	1880	1.355	3995850	326791	
Tetracosane	1860	1.317	3892177	58641	
Tetraethylene gl...	1820	1.829	3882756		
Tetracosane	1968	1.371	3854000		
Dotriacontane	2180	1.605995	3347451		
Tritriacontane	2224	1.675	3150766		

- Results from suspect screening analysis (SSA) testing of baby onesies
- There is a need to distinguish between the chemicals in a product, and those which may emit under normal use conditions

U.S. EPA Office of Research and Development unpublished data

Challenges and emerging research

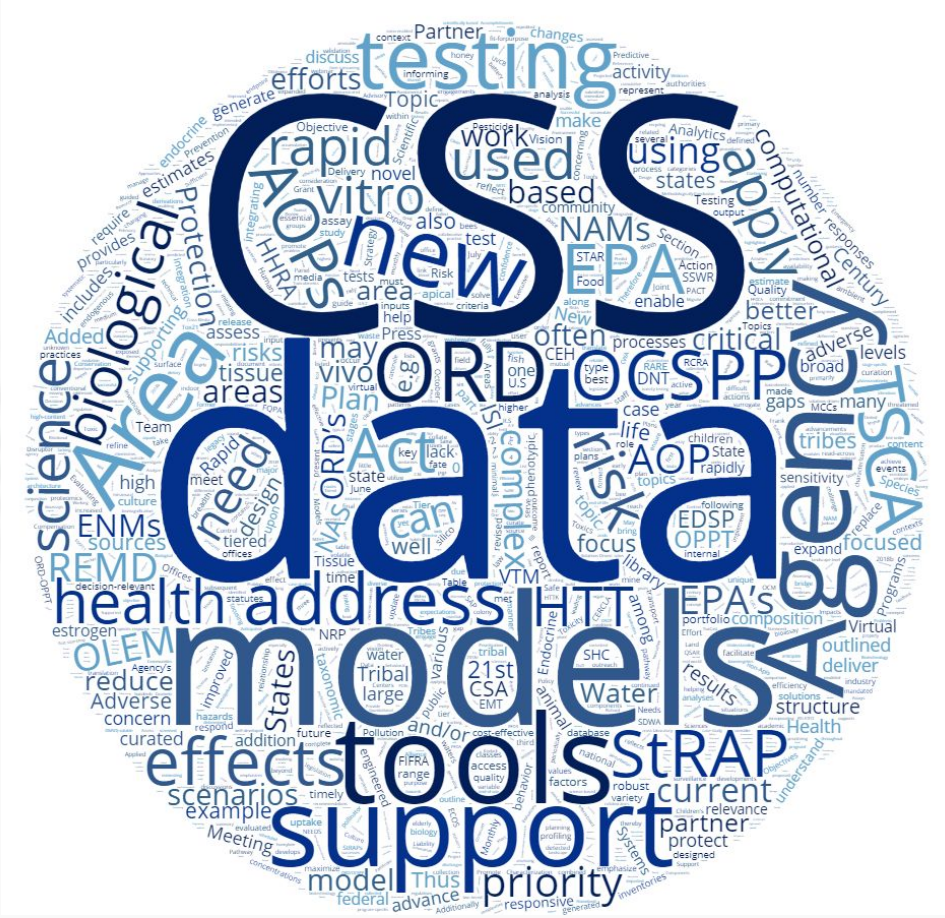
- Chemical identification and naming (Grulke et al. 2019)
- Consumer product composition
  - Data access, updates, and transparency
  - Disclosed vs. nondisclosed ingredients (including proprietary mixtures and contaminants)
  - Active vs. inactive ingredients
  - Mixtures in the indoor environment
- Data gaps in emissions parameters needed for modeling
  - Challenges with measuring emissivity (lab work is expensive and time consuming)
  - Differences in emissivity from different substrates for the same chemical
  - Differences in composition of products vs. chemicals which may be emitted

Acknowledgments

U.S. Environmental Protection Agency

Office of Research and Development

Chemical Safety for Sustainability Research Program



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John Wambaugh

Todd Luxton

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