

High-throughput Occupational Exposure Efforts at US EPA

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HT Pathway Predictions are Needed for Decision Workflows

- Human exposure pathway predictions for thousands of chemicals are currently integrated into working approaches for identifying potential candidates for prioritization under TSCA
 - Consumer, dietary, and ambient predictions currently integrated into consensus predictions
- Efforts are underway to incorporate high-throughput ecological exposure predictions for integration with ecological hazard data
- It is also ultimately desirable to predict occupational exposures in a high-throughput manner for use in such workflows
 - TSCA directs EPA to address potentially exposed or susceptible sub-populations, defined as a group of individuals within the general population identified by the Administrator who, due to either greater susceptibility or greater exposure, may be at greater risk than the general population of adverse health effects from exposure to a chemical substance or mixture, such as infants, children, pregnant women, workers, or the elderly.



September 27, 2018 Office of Chemical Safety and Pollution Prevention

A Working Approach for Identifying Potential Candidate Chemicals for Prioritization





Occupational Exposure

- EPA has made great strides in evaluating exposure models for the general population which can assess thousands of chemicals quickly
- Occupational exposure requires considering different exposure scenarios and different chemicals workers are exposed to across many different occupations
- Potential exposures often classified by different occupational classes





Consensus Exposure Modeling

- Multiple high-throughput exposure models can be run for a given population assuming general consumer, dietary, and far-field exposures
- Results are coupled through the Systematic Empirical Evaluation of Models (SEEM) framework





Path to Occupational Exposure





ChemSTEER

- Developed by EPA to estimate workplace exposures and environmental releases
- Requires manual input of information
- 6 dermal exposure models
 - 1-hand dermal contact with liquid
 - 2-hand dermal contact with liquid
 - 2-hand dermal immersion in liquid
 - Direct 2-hand dermal contact with solids
 - 2-hand dermal contact with container surfaces
 - User defined
- 11 inhalation exposure models
 - Small volumes handling
 - PEL-limiting for substance specific particulates
 - Total PNOR PEL-limiting
 - Respirable PNOR PEL-limiting
 - Automobile OEM Spray Coating
 - Automobile Refinish Spray Coating
 - Automobile Spray Coating
 - UV Roll Coating
 - User defined
 - Mass balance
 - PEL-limiting for substance specific vapors

Chemical-agnostic Models





CLOET

High-throughput Command Line Occupational Exposure Tool (CLOET) a command line tool that allows calculation of ChemSTEERv3.0 exposure models.

Written in base Python 3.0, so it depends on no external packages.

Multiple scenarios for each model have been run and tested against ChemSTEER GUI to test for model fidelity.

```
>>> import cloet
>>> e_derm = (cloet.dermal
                         .one_hand_liquid_contact(Yderm=0.5))
>>> e_derm.inputs
{'ED': 1,
    'NWexp': 1,
```

```
'Dexp': 561.75}
```

'APDR': 8.025,

'NS': 1, 'EY': 40,

'BW': 70,

'S': 535,

'FT': 1,

{'NW': 1,

'Qu': 2.1,

'Yderm': 0.5}

>>> e derm.outputs

'LADD': 0.012563600782778865,

'ADD': 0.021986301369863015,

'ATc': 70, 'AT': 40,



Chemical Agnostic ChemSTEER Models

DERMAL MODELS

INHALATION MODELS



Concentrations were varied from 0.1 to 1 for all chemical agnostic models

Office of Research and Development Center for Computational Toxicology and Exposure

Phillips et al, in preparation



UNITED STATES DEPARTMENT OF LABOR

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Occupational Safety and Health Administration

CONTACT US FAQ A TO Z INDEX ENGLISH ESPAÑOL

SEARCH OSHA

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OSHA ✓ STANDARDS ✓ TOPICS ✓ HELP AND RESOURCES ✓

Data & Statistics / Chemical Exposure Health Data

Chemical Exposure Health Data

OSHA compliance officers often take industrial hygiene samples when monitoring worker exposures to chemical hazards. Many of these samples are submitted to the Salt Lake Technical Center (SLTC) for analysis. The sampling results included on this web page represent the records of the SLTC sampling information system from 1984 forward. They include data on personal, area, and bulk samples for various airborne contaminants. All inspection sampling results will be included here once the case is closed. OSHA does not publicly disclose information from the following types of cases: open inspections and citations currently under contest or under appeal to the Occupational Safety and Health Review Commission or the U.S. Courts of Appeals. After litigation has concluded, the sampling data from the related inspection will be added at the next scheduled update. OSHA updates the data on this web page semi-annually in January and July.

OSHA

by year

Personal sampling results represent the exposure to the individual who was actually wearing a sampling device. Area samples are taken in a fixed location and results may represent the potential risk from airborne contaminants or physical agents to workers in that area. Bulk

samples we

conjunction

Please note values may

OSHA Chemical Exposure Health Data

- Data available from 1989 2018
- One record is one sample taken from one work site for one chemical
- Inhalation Samples: 1.3 million samples; ~1000 substances; both area and personal sampling
- Dermal Samples: ~200,000 samples, ~70 substances, dermal wipes



Organizing OSHA Data

- Standardized and unified all years into one dataset
- Cleaned missing or unlabeled data
- Converted old SIC/NAICS codes to 2017 NAICS codes
- Converted all air samples to mg/m³
- Matched OSHA substance names to substances in DSSTox database by synonym searching on the EPA CompTox Dashboard.
- Substances that returned no match were searched manually in PubChem for synonyms





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Caveats to OSHA Data

- OSHA collected multiple measured values in a single sampling effort; to capture a "worst case" scenario, these records were aggregated to the maximum measured value (for example, measurements of 0, 0, and 12 mg/m³ in a single inspection are aggregated to 12 mg/m³ for that inspection)
- OSHA data is <u>not</u> a random sampling of every workplace. These sampling efforts typically only occur when someone is suspicious of a violation in a workplace. For this reason, the measurements can tend to be higher than average both in concentration and in frequency of detection.
- Concentrations for naturally occurring compounds in air (CO₂, O₂, N₂, etc.) are included in measurements even though they typically do, and should, exist in environments at high concentrations.



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Two-Stage Model

Using Bayesian Hierarchical Regression, we can construct a model where, knowing nothing about a chemical other than its structure, we can predict:

- the likelihood of a chemical being detected by OSHA's air measurement methods
- they likely concentration of chemical detected in an air sample





Bayesian Hierarchical Models

- Bayesian Hierarchical Regression allows us to organize our predictions (either detect/non-detect or concentration) by NAICS Sector and/or Subsector
- When data is lacking, at the Subsector level, we can aggregate up to the Sector prediction
- OPERA physicochemical property distributions across NAICS sector and subsectors are included as input distributions to the models in addition to OSHA data







Physicochemical Effects

Substances are more likely to be *detected* in the air of a workplace with

- Low
 - Boiling Point
- High
 - Octanol-water Coefficient (logP)
 - Henry's law constant (loghl)
 - HPLC retention time (rt)

<u>Note</u>: the properties listed are all *predicted* properties from the OPERA suite.

Minucci et al, in preparation



Detection and Concentration by NAICS sectors



Center for Computational Toxicology and Exposure



Support Activities for Agriculture and Forestry Furniture and Related Product Manufacturing Personal and Laundry Services Printing and Related Support Activities Apparel Manufacturing Chemical Manufacturing Administration of Environmental Quality Programs Specialty Trade Contractors Nonstore Retailers Paper Manufacturing Miscellaneous Manufacturing Fabricated Metal Product Manufacturing Repair and Maintenance Textile Mills Animal Production and Aquaculture Transportation Equipment Manufacturing Real Estate Motor Vehicle and Parts Dealers Textile Product Mills Computer and Electronic Product Manufacturing Primary Metal Manufacturing Beverage and Tobacco Product Manufacturing Wood Product Manufacturing Nonmetallic Mineral Product Manufacturing Rental and Leasing Services Sporting Goods, Hobby, Musical Instrument, and Book Stores Food Manufacturing Machinery Manufacturing Electrical Equipment, Appliance, and Component Manufacturing Hospitals Educational Services National Security and International Affairs Wholesale Electronic Markets and Agents and Brokers Merchant Wholesalers, Durable Goods Ambulatory Health Care Services Building Material and Garden Equipment and Supplies Dealers Miscellaneous Store Retailers Professional, Scientific, and Technical Services Merchant Wholesalers, Nondurable Goods Support Activities for Transportation General Merchandise Stores Petroleum and Coal Products Manufacturing Furniture and Home Furnishings Stores Construction of Buildings Nursing and Residential Care Facilities Telecommunications Plastics and Rubber Products Manufacturing Water Transportation Social Assistance Air Transportation Justice, Public Order, and Safety Activities Warehousing and Storage Amusement, Gambling, and Recreation Industries Rail Transportation Waste Management and Remediation Services Accommodation Truck Transportation Executive, Legislative, and Other General Government Support Clothing and Clothing Accessories Stores Crop Production Postal Service Administrative and Support Services Couriers and Messengers Transit and Ground Passenger Transportation Support Activities for Mining Food Services and Drinking Places Motion Picture and Sound Recording Industries Administration of Human Resource Programs Admin., Support, Waste Manage. and Remediation Services Utilities Health and Personal Care Stores Administration of Economic Programs Credit Intermediation and Related Activities Food and Beverage Stores

Leather and Allied Product Manufacturing

Predictions by NAICS Subsectors

Highest likelihood of detection

Environmental Protection

Agency

- Leather and Allied Product Manufacturing
- Support Activities for Agriculture and Forestry
- Furniture and Related Products Manufacturing
- Lowest likelihood of detection
 - Food and Beverage Stores
 - Credit Information and Related Activities
 - Administration of Economic Programs

Leather and Allied Product Manufacturing		· · · · · · · · · · · · · · · · · · ·
Support Activities for Announcementation		
Eurpiture and Polated Product Manufacturing		
Personal and Laurday Conving	1	
Personal and Laundry Services	1	
Printing and Related Support Activities	1 *	
Apparel Manufacturing	1	
Chemical Manufacturing	• •	_ → _
Administration of Environmental Quality Programs	· · · · · · · · · · · · · · · · · · ·	
Specialty Trade Contractors		—
Nonstore Detailers		· · ·
Danas Manufacturing		
Paper Manufacturing		
Miscellaneous Manufacturing	1 *	
Fabricated Metal Product Manufacturing	•	→
Repair and Maintenance	• •	•
Textile Mills		
Animal Production and Aquaculture		
Transportation Equipmont Manufacturing		
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Motor Vehicle and Parts Dealers	1 *	
Textile Product Mills	1	
Computer and Electronic Product Manufacturing	• •	l —•- I
Primary Metal Manufacturing	4 🔶	I − ●−
Beverage and Tobacco Product Manufacturing		
Weed Deduct Manufacturing		
Neemetallia Misseed Product Manufacturing		
Nonmetanic Mineral Product Manufacturing		
Rental and Leasing Services	1	
orting Goods, Hobby, Musical Instrument, and Book Stores	1	
Food Manufacturing	1 	
Machinery Manufacturing	4 🔶	l <u>-</u>
rical Equipment, Appliance, and Component Manufacturing	4 🔺	l <u> </u>
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Hospitais		
Educational Services		
National Security and International Affairs	1	
Wholesale Electronic Markets and Agents and Brokers	· · · · · · · · · · · · · · · · · · ·	
Merchant Wholesalers, Durable Goods	4	
Ambulatory Health Care Services	· · · ·	
ding Material and Garden Equipment and Supplies Dealers		i <u>-</u>
Missellanders Character Equipment and Supplies Dealers		
Miscellaneous Store Retailers		
Professional, Scientific, and Technical Services	1	
Merchant Wholesalers, Nondurable Goods	l	
Support Activities for Transportation	4 	
General Merchandise Stores		
Petroleum and Coal Products Manufacturing		
Eurpiture and Home Eurpichings Stores		
Furniture and nome Furnishings Stores		
Construction of Buildings		
Nursing and Residential Care Facilities		
Telecommunications		
Plastics and Rubber Products Manufacturing	• •	
Water Transportation	· · · · · · · · · · · · · · · · · · ·	
Social Assistance	· · · · · · · · · · · · · · · · · · ·	
Social Assistance		
All Transportation		
Justice, Public Order, and Safety Activities		
Warehousing and Storage		
Amusement, Gambling, and Recreation Industries	1	
Rail Transportation	1	
Waste Management and Remediation Services	1	
Accommodation	· · · · · · · · · · · · · · · · · · ·	l I
Truck Transportation		l
utive Legislative and Other General Government Support	I	
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Clothing and Clothing Accessories Stores		
Crop Production		
Postal Service	1	
Administrative and Support Services	1	
Couriers and Messengers	· · · · · · · · · · · · · · · · · · ·	
Transit and Ground Passenger Transportation		
Support Activities for Mining		
FOOD SERVICES and Uniperiod Process		
Motion Disture and Second Depending Is dustrian		
Administration of Living Recording Industries		
Administration of Human Resource Programs	1	
Admin., Support, Waste Manage. and Remediation Services	1	
Utilities	· · · · · · · · · · · · · · · · · · ·	
Health and Personal Care Stores	Ⅰ	I −−− ● −−−
Administration of Economic Programs	• •	
Credit Intermediation and Palated Activition		
Ered and Revenue Change		
Food and Beverage Stores		
	0.0 0.2 0.4 0.6 0.8 1.0	-1 0 1 2 3
	Probability of detection	Air concentration (log mg/m2)
	FIODADILLY OF DELECTION	An concentration (log mg/m3)

Environmental Protection Agency

Predictions by NAICS Subsectors

- Highest likelihood of detection
 - Leather and Allied Product Manufacturing
 - Support Activities for Agriculture and Forestry

Elec

Bui

Exe

- Furniture and Related Products Manufacturing
- Highest predicted concentration (if detected)
 - Support Activities for Mining
 - Social Assistance
 - Leather and Allied Product Manufacturing



True Positive and False Negative Concentration Predictions of Test Set



log₁₀[Predicted Air Conc. (mg/m³)]





Next Steps

- Use detect/non-detect and concentration models to predict concentration of chemicals
- Use QSUR-models to predict functional use (technical function) and sector of use of chemical
- Use sector of use and concentration to choose which ChemSTEER models apply to which chemicals in which sectors and get exposure estimates





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