Environmental Release and Occupation Exposure Models Used in Chemical Risk Evaluation

William M. Barrett, Ray Smith, David Meyer, Sudhakar Takkellapati, and Michael A. Gonzalez*

U.S. Environmental Protection Agency, Center for Environmental Solutions & Emergency Response
Land Remediation & Technology Division, 26 W. Martin Luther King Dr., Cincinnati, OH 45268

Office of Research and Development
Center for Environmental Solutions & Emergency Response
Land Remediation & Technology Division

EPA United States Environmental Protection Agency

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Overview

- Review of Chemicals under TSCA.
- What Are Generic Scenario and Exposure Scenario Documents.
- Current Modeling of Occupational Emissions and Environmental Releases.
- Approaches to Simplify Human Exposure Modeling.

Overview of Toxic Substances Control Act (TSCA)

- Existing Chemicals:
  - Compile, keep current, and publish a list of all chemicals substances that are manufactured or processed, including imported, in the United States.
  - Currently, the TSCA inventory includes over 86,000 unique chemical substances.
- New Chemicals:
  - Not on the TSCA Chemical Substances Inventory.
  - Manufacturers or importers submit a Premanufacturing Notice (PMN).
  - EPA review to determine if the chemical substances pose an unreasonable risk prior to the chemical being manufactured or imported.
- TSCA requires the US EPA to conduct a full life-cycle risk assessment, including evaluations of the chemistry, environmental fate, engineering, exposure, and human and ecological health assessments of a substance.

https://www.epa.gov/tsca-inventory/about-tsca-chemical-substance-inventory

EPA's Timeline for Chemical Review

- US EPA has 90 days to review a PMN or SNUN
  - Render an affirmative determination.
- Company files a Notice of Commencement of Manufacture or Import (NOC) within 30 days of first manufactured or imported.
- New chemicals are added to the TSCA inventory following receipt of the NOC.
- Between June 22, 2016, and November 1, 2022, the US EPA completed reviews of 1,839 Pre-Manufacture Notices (PMNs), Microbial Commercial Activity Notices (MCANs), and Significant New Use Notices (SNUNs) - average of over 25 new chemical review cases completed per month.
- On March 1, 2022, the US EPA had a total of 397 active PMN or SNUN cases under review in the risk assessment, risk characterization, or regulatory decision or action development phase. Of those, 289 cases were in the risk assessment phase of the review process.

USEPA, TSCA New Chemical Determinations: A Working Approach for Making Determinations under TSCA Section 5. OPPT, Ed. 2019
https://www.epa.gov/reviewing-new-chemicals-under-toxic-substances-control-act-tsca/statistics-new-chemicals-review#stats

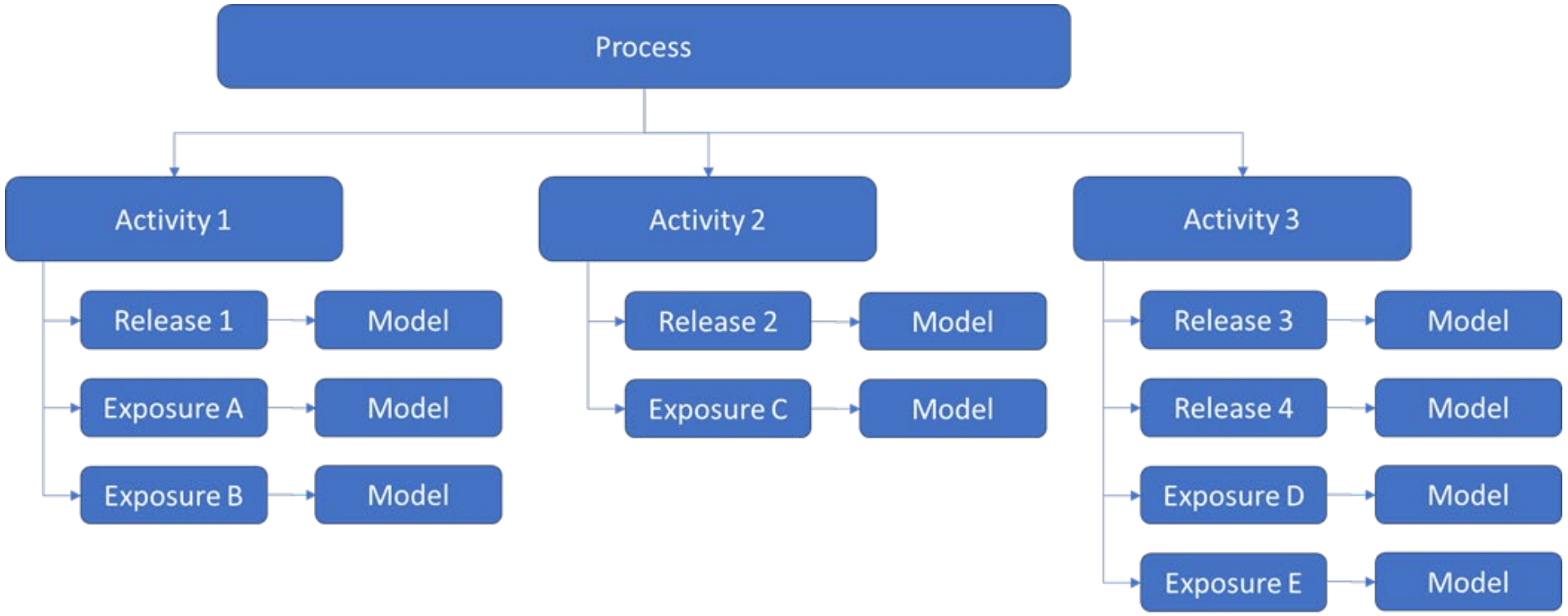
Generic Scenarios

- The EPA develops and uses GS documents to address data gaps in chemical risk assessments performed under TSCA.
- A set of conditions about sources, pathways, production processes and use patterns that quantify the emissions (or releases) of a chemical from production, formulation, processing, private use (or use in the household) and recovery/disposal into water, air and solid waste.
- Provide estimates of environmental releases and occupational exposures associated with chemical uses across industries.
- Releases are modeled based upon activities (such as emptying a drum) performed within an industry.
- Framework for collection of models for exposure assessment associated with the industry. Cumulative emissions models.

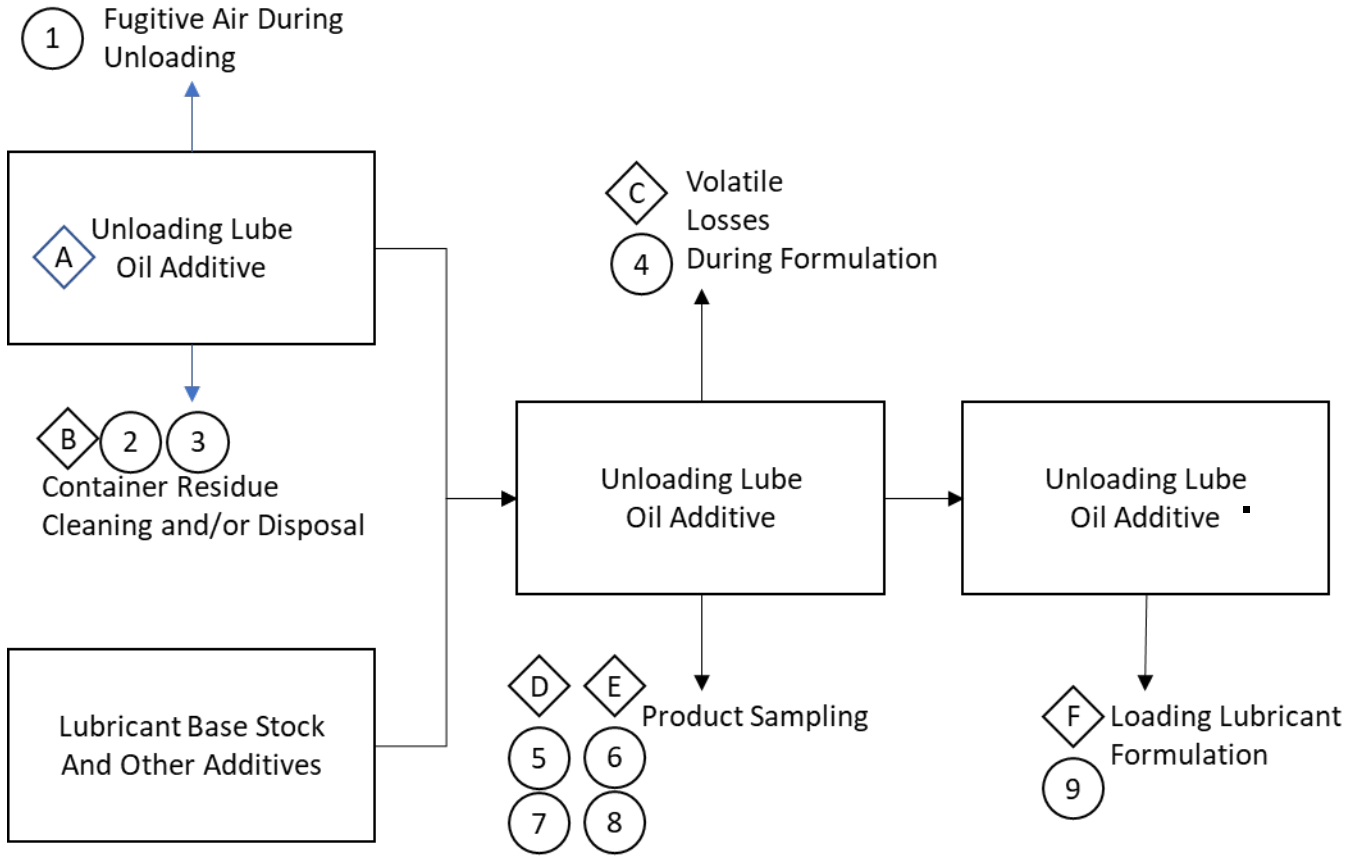
Components of a Generic Scenarios

- A description of the industry or use.
- A description of the types of substance used and their function in the industry area.
- Information on the scale or size of operations in the industry area.
- Identification of the points of release in the use area and estimates of the amounts of substances released at these points.
- Information on emission control methods for the industry.
- Instructions on how to use the information in the document, and examples of calculations.

Generic Scenario Modeling



Activities, Occupational Exposures, and Environmental Releases for Chemical Additives Used in Automotive Lubricants



Environmental Releases:

1. Transfer operation losses of volatile chemicals to air
2. Container residue losses to water, incineration, or landfill
3. Open surface losses of volatile chemicals during container cleaning to air
4. Vented losses of volatile chemicals to air during blending
5. Open surface losses of volatile chemicals to air during product sampling
6. Product sampling wastes to water, incineration, or landfill
7. Equipment cleaning losses to incineration or landfill
8. Open surface losses of volatile chemicals during equipment cleaning to air
9. Transfer operation losses of volatile chemicals to air

Occupational Exposure:

A. Inhalation (volatiles only) and dermal exposures during container unloading
B. Inhalation (volatiles only) and dermal exposures during container cleaning
C. Inhalation (volatiles only) exposure during formulation
D. Inhalation (volatiles only) and dermal exposures during product sampling
E. Inhalation (volatiles only) and dermal exposures during equipment cleaning
F. Inhalation (volatiles only) and dermal exposures during container loading

Note: lube oil additives and lubricant base stock/other additives

USEPA, Emission Scenario Document on Chemical Additives Used in Automotive Lubricants. 2016

ChemSTEER

- Compilation of USEPA models used for screening level assessments.
- ChemSTEER was initially developed in 2003/2004 timeframe and was updated in 2015.
- The methods and models used in ChemSTEER are largely from the Chemical Engineering Branch's (CEB) Manual for Preparation of Engineering Assessments (1991) and other US EPA models, and the CEB's compilation of GS documents.
- Currently, ChemSTEER compatibility is a consideration in the development of GS or ESD.
- We reviewed the models in ChemSTEER models to provide an understanding of how the decision-making framework is implemented.

USEPA ChemSTEER-Chemical Screening Tool for Exposures and Environmental Releases. https://www.epa.gov/tsca-screening-tools/chemsteer-chemical-screening-tool-exposures-and-environmental-releases.

Regulatory Models

- Occupational exposure and environmental release models:
  - Estimate facility specific releases and exposures.
  - Provide insight into the risk associated with a specific chemical to develop an effective regulatory approach.
- Regulatory risk assessment
  - Estimate exposures for loosely specified scenarios reflecting the variability of conditions of use where the substance is used or processed.
  - Specifics of the condition of use that underly any exposure scenario must be broad enough to cover conditions that may be encountered across the spectrum of workplaces where the chemical may be used.
  - These site-specific parameters will vary significantly across a facility or industry, resulting in highly variable exposures and releases across all the workplaces where the exposure scenario occurs.

Cherrie, J. W.; et al, (2020)., *International Journal of Environmental Research and Public Health*.

Model Tiers

- Tier 1
  - Relatively simple.
  - Designed to identify high risk chemicals for more detailed (higher tier) analysis.
  - Key consideration: Simplify complicated problems for the scenario in question.

- Tier 2
  - Combine mechanistic models with measured exposure values.
  - Measured data used to parameterizing the mechanistic model.
  - Bayesian approach incorporates uncertainty and variability to improve model estimates.

- No matter how many tiers, increased accuracy of the exposure assessment comes at a price in terms of the complexity of the assessment and the time required to gather additional information.

Tielemans, E.; et al, (2011) Annals of Occupational Hygiene.
Money, C., (2018) Environmental Science: Processes & Impacts.
Tielemans, E.; (2007) Journal of Exposure Science & Environmental Epidemiology.

Modeling Challenges

- Model variability and uncertainty are challenges associated with the development of occupational exposure models.
  - Variability arises from differences in people and circumstances that cannot be altered without changing the scenario.
  - Uncertainty results from lack of knowledge about the situation being modeled and can be reduced by obtaining additional data.
- Regulatory exposure evaluations have significant data gaps. There is an increasing need for fate and exposure modeling to fill these gaps.
- Challenges still remain around creating a common scientific framework for exposure assessments, improving the coordination of the regulatory process, and improving incorporation of exposure science in chemical risk evaluation.

Tielemans, E, et al, (2007) Journal of Exposure Science & Environmental Epidemiology.
Bonnell, M. A.; et al., (2018) Environmental Science: Processes & Impacts
Bruinen de Bruin, Y.; et al, (2021) Journal of Exposure Science & Environmental Epidemiology

Opportunities to Improve Models

- High-Throughput (HT) Modeling:
  - Goal: find ways to apply existing theory and models to large groups of chemicals.
  - Example: grouping chemicals by use and general exposure route models.

- Life Cycle Approach
  - Develop a set of standardized activities for each life cycle stage, such as manufacturing, processing, use, and disposal.
  - Need to standardize the approach and prepare for an assessment of releases useful for occupational exposures.

Dealing with Uncertainty and Variability

- Typical approach in exposure assessment is to focus on the worst-case scenario
  - Hides valuable information related to the uncertainty of the value.
  - Provides no knowledge about the relative range of the prediction.
- Known variability should be addressed through separate models considering the different circumstances that represent the system.
- Bayesian allow expert judgement to be informed by model results, updated with sparse historical monitoring data.
- Monte Carlo-type approach could be used that varies model parameters and obtains the mean, median, and 90th percentile of a distribution to quantify conservative exposure or release estimates for use in decision making.

Jayjock, M. A., Uncertainty Analysis in the Estimation of Exposure. American Industrial Hygiene Association Journal 1997, 58 (5), 380-382.
Cullen, A. C.; Frey, H. C.; Frey, C. H., Probabilistic Techniques in Exposure Assessment: A Handbook for Dealing with Variability and Uncertainty in Models and Inputs. Springer US: 1999.

Conclusions

- Current approach uses Tier 1 occupational exposure and environmental release models developed in the 1980s and 1990s.
- Models presented in GS and ESD cover expected environmental releases and occupational exposures during manufacturing and commercial use but do not include other lifecycle stages for the chemical.
- There is a need to consider the uncertainty of release and exposure estimates.
- Additional data sources should be identified or obtained to improve the occupational exposures and environmental releases models presented in the GS/ESD.
- “What are the risk-based concentrations in environmental media protective of human and ecological health outcomes?”

von Stackelberg, K.; Williams, P. R. D., Evolving Science and Practice of Risk Assessment. Risk Analysis 2021, 41 (4), 571-583.

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Thank you for your attention!
Any Questions?