TSCA EXPOSURE WORKSHOP
Deterministic Modeling Approaches

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May, 2024

PRESENTATION OUTLINE

1. Deterministic models – description
2. Application of Deterministic Models
3. Common EPA Deterministic Models
4. Use of Deterministic Models in New Chemicals Exposure Assessments
5. Use of Deterministic Models in Existing Chemical Assessments
   - Example: Dermal Exposure to Volatile Liquids Model

Deterministic Models

- Deterministic models have a single output (or set of outputs) for a given input (or set of inputs).
- These differ from probabilistic models, which are a type of stochastic model. Probabilistic models incorporate input parameter probability distributions to output a distribution of potential results.
- EPA's exposure models can utilize both deterministic or probabilistic approaches, depending on whether the model input parameters have a single value or have distributions, as discussed above.

Applications of Deterministic Models

- The choice to use a deterministic modeling approach is dependent on input parameter data availability and the end use application of the model.
- Data Availability:
  - EPA may have data that specifically indicates that inputs do not vary such that the model outputs are set at single deterministic value; or
  - EPA may suspect variability in the inputs but not have the data available to incorporate that variability into the model.
- End-Use Application:
  - The application of the model may not require incorporating of input variability and probability distributions if only a single deterministic result is desired (e.g., screening-level assessments to estimate “worst-case” scenarios).

Common EPA Deterministic Models

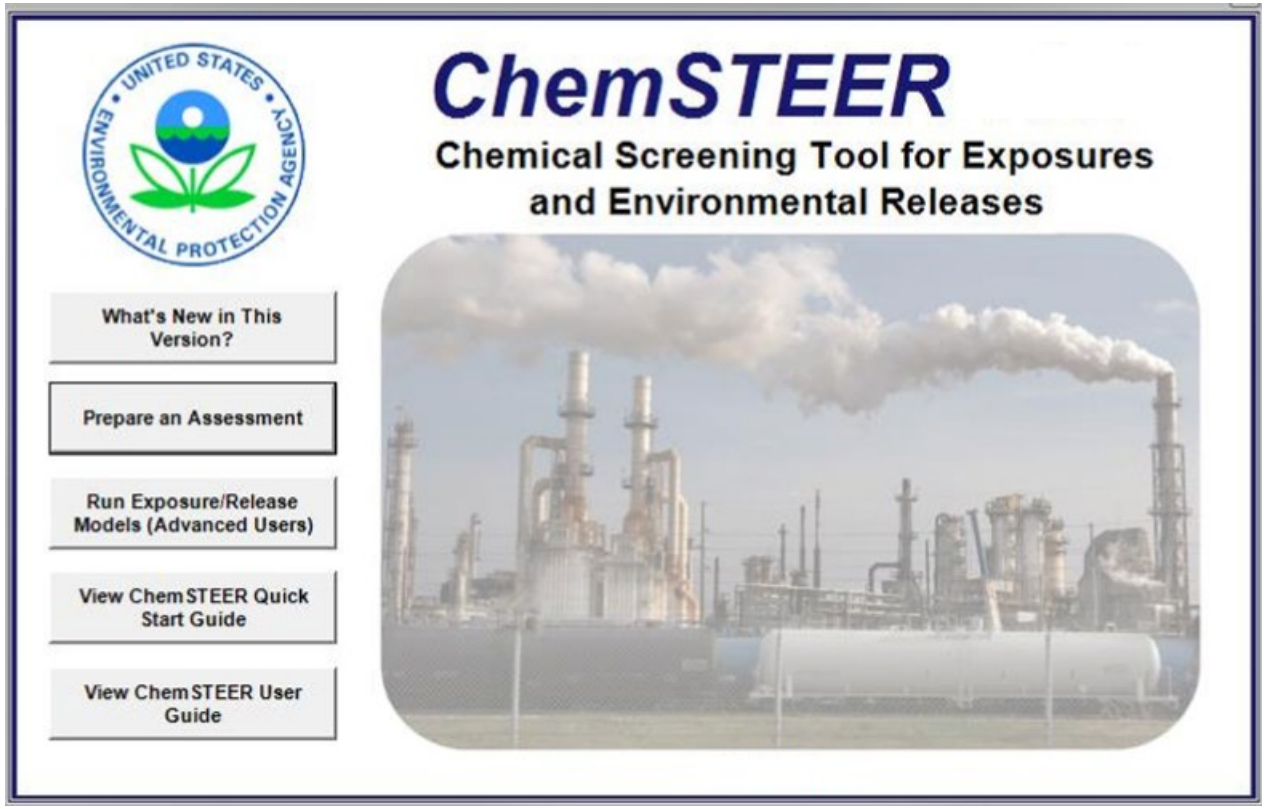
- EPA/OAQPS AP-42 Loading Model
- EPA/OPPT Mass Transfer Coefficient Model
- EPA/OPPT Penetration Model
- EPA/OPPT Mass Balance Inhalation Model
- EPA/OPPT Small Volume Handling Model
- All EPA/OPPT Dermal Exposure Models
- Tank Truck and Railcar Loading and Unloading Release and Inhalation Exposure Model

Refer to the ChemSTEER User Guide for explanation of these models.

Refer to EPA's risk evaluations for perchloroethylene and 1-bromopropane, among others, for explanation of this model.

Use of Deterministic Models in New Chemical Assessments

- EPA most often applies deterministic models in new chemical assessments.
- New chemical assessments typically utilize the publicly-available software ChemSTEER to estimate environmental releases and occupational exposures.
- Most of the deterministic models mentioned on the previous slide are programmed into ChemSTEER.



ChemSTEER software is available for download on [EPA's website](#).

Deterministic Model in ChemSTEER – EPA/OAQPS AP-42 Loading Model

Activity: (1) Run Models

Model: EPA/OAQPS AP-42 Loading Model

Model Equation: DR (kg/site-day) = (G × 3600 × OHa) / 1000

Vapor Release Mechanism: Displacement of air containing chemical vapor

☑ Enable Model Parameters for Output 1 — Typical

☑ Enable Model Parameters for Output 2 — Worst Case

Basis: EPA/OAQPS AP-42 Loading Model.

Parameters:

Parameter	Origin 1	Value 1	Type 2	Origin 2	Value 2	Units
MW: Molecular Weight	User Specified	100	Non-default	User Specified	100	g/mol
NS: Number of Sites	User Specified	1	Non-default	User Specified	1	sites
Oha: Operating Hours for the Acti	User Specified	8	Non-default	User Specified	8	hours/day
r: Container Rate	User Specified	60	Non-default	User Specified	60	containers/h
R: Universal Gas Constant	Model Parm	82.05	Constant	Model Parm	82.05	atm cm3/gmc
T: Temperature	Model Parm	298	Default	Model Parm	298	K
Vc: Volume Capacity of container	User Specified	55	Non-default	User Specified	55	gal/container
VP: Vapor Pressure	User Specified	19.5	Non-default	User Specified	19.5	torr

OK Cancel

Model input parameters, with deterministic (static) values

Use of Deterministic Models in Existing Chemical Assessments

- EPA prefers the use of probabilistic modeling in existing chemical risk evaluations; however, EPA may occasionally use deterministic models depending on input parameter data availability and the end-use application, as previously discussed.
- The Engineering Assessment Predictability Tables indicate where EPA has used deterministic modeling in published risk evaluations thus far. Some examples include (from first 10 chemicals):
  - Tank Truck and Railcar Loading and Unloading Release and Inhalation Exposure Model
  - Dermal Exposure to Volatile Liquids Model

Example: Deterministic Model in Existing Chemicals Risk Evaluations

Dermal Exposure to Volatile Liquids Model

$$D_{exp} = S \times \frac{(Q_u \times f_{abs})}{PF} \times Y_{derm} \times FT$$, with the following parameters:

- S, the surface area of contact: 535 cm^2 (central tendency) and 1,070 cm^2 (high-end)
- Q_u, the quantity remaining on the skin: 1.4 mg/cm^2-event (central tendency) and 2.1 mg/cm^2-event (high-end).
- Note:
  - Values of S and Qu were modified in 2000 after Peer Review of Occupational Exposure Dermal Method.
  - Values of S were modified again in 2013 with updated Exposure Factors Handbook
  - Combinations of S and Q characterized as representative of central tendency and high-end were established in the 1st 10 RE's
- F_{abs} = fraction of applied mass that is absorbed (%)
- PF, the fraction of chemical that penetrates the glove (protection factor): PF = 1 without the use of gloves.
- Y_{derm}, the weight fraction of the chemical of interest in the liquid: EPA will assess a unique value of this parameter for each occupational scenario or group of similar occupational scenarios. (1.0 for 1,1-DCA and all other chemicals listed above)
- FT, the frequency of events: 1 event per day.