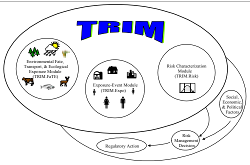

Evaluation of the TRIM.FaTE multi-media model: A mercury case study

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1. Abstract

TRIM.FaTE, the Fate, Transport and Environmental Exposure module of USEPA's Total Risk Integrated Methodology is a multimedia compartmental model designed to support needs of the Agency in considering non-air impacts of hazardous air pollutants. As part of model evaluation, we have recently employed it in a case study involving a source of mercury air emissions, and distribution and accumulation of mercury species in surrounding environmental media and biota. In addition to evaluating model performance and parameter uncertainty, the case study is being used to facilitate the preparation of users's guidance for TRIM.FaTE. Representative wildlife and aquatic biota resident to the area were included in the modeled scenario. Initial concentrations of elemental, divalent and methyl mercury in media and biota were set based on preliminary runs using meteorological data for the full run, with current reported background as the only source of mercury. Preliminary simulations of reduced scenario complexity were used to troubleshoot model parameters, algorithms and linkages prior to full scenario runs. This troubleshooting step also highlighted issues important to assessing model uncertainty and particularly relevant to designing a simulation, which will be discussed in the user's guidance document. Some issues (e.g., meteorological time steps) may arise with other multimedia models, while others (e.g., designing parcel layout and compartment linkages) may be particular to TRIM.FaTE. The full case study was run simulating facility operation contributing air emissions of mercury for 30 years. Only the initial media concentrations, air boundary conditions, and these source emissions were included. For general gauging of model outputs, literature reported mercury levels in various media and biota, and limited measurement data available near the source were consulted. Given the scope and limitations of the case study simulation, model outputs generally indicate comparability with these values. An analysis of uncertainty and variability was performed to assess some aspects of model and parameter uncertainty. Other modeling aspects (e.g., related to design of the model scenario) were recognized as additional sources of uncertainty to model outputs that will require separate analysis. Further, results of the 30 year run and associated uncertainty analysis, are also being compared to a comparable simulation being performed using another USEPA multimedia model. The Multi-media, Multi-receptor, Multi-pathway Risk Analysis (3MRA) modeling system, using a linked media approach, is being applied to the same site. Of interest in the model comparison are the influence on predictive endpoints of different modeling approaches and consideration of issues including uncertainty analysis, computational resource requirements, data requirements, and problem conceptualization.

2. TRIM.FaTE is one of the three modules within the Total Risk Integrated Methodology (TRIM)

Fate, Transport & Ecological Exposure Module (TRIM.FaTE) ..

- is a time series mass balance model that accounts for the movement of a chemical(s) through a system of discrete compartments (e.g., media, biota) representing possible locations in the physical and biological environments of the modeled ecosystem.
- is intended for air pollutants with important non-inhalation exposures.
- generates both media concentrations relevant to human pollutant exposures and exposure estimates relevant to ecological risk assessment.

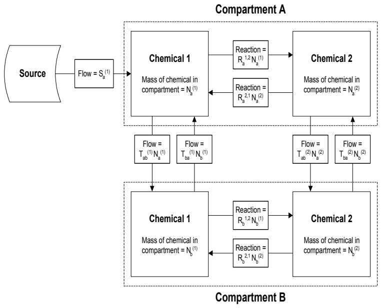
Exposure Event Module (TRIM.Expo) ...

- Assesses human exposures by tracking the activities of population groups and their inhalation and ingestion through time and space.
- Can receive input from TRIM.FaTE or air quality models or monitoring data.

Risk Characterization Module (TRIM.Risk) ...

- Calculates human health and ecological risk metrics.
- Documents model inputs & assumptions.
- Displays results.

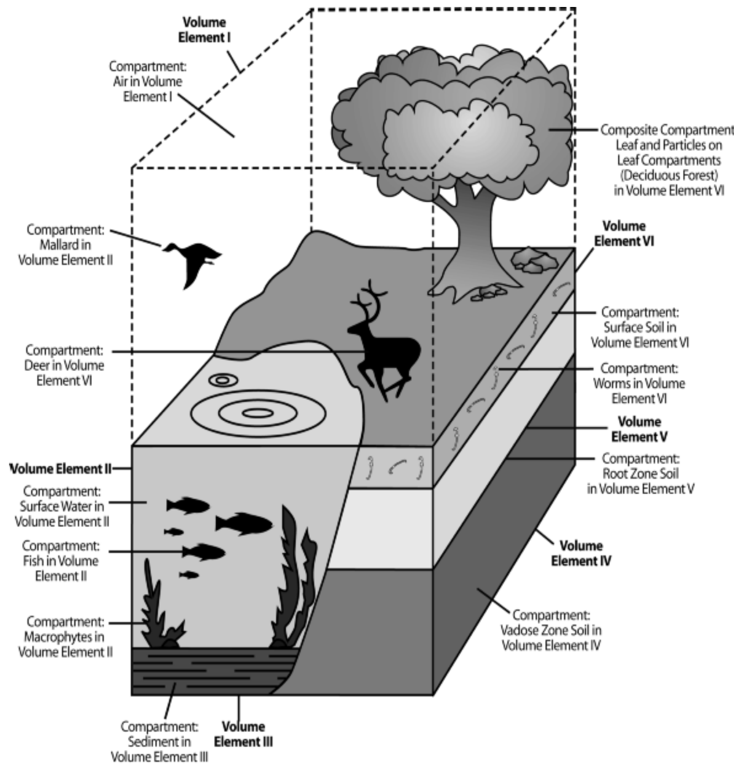
3. TRIM.FaTE is a truly coupled multimedia model



- Transfer of pollutants among **multiple media** and exposure of biota via **multiple pathways.**
- **Transparent approach** embodied in an easily accessible algorithm and input value library.
- **Flexibility of spatial & temporal scales, time step**, and in the definition of compartments & linkages.
- **Uncertainty/Variability** capabilities include both sensitivity and Monte Carlo.

4. TRIM.FaTE Modeling System

TRIM.FaTE relies on a system of parcels, volume elements & compartments of various type.

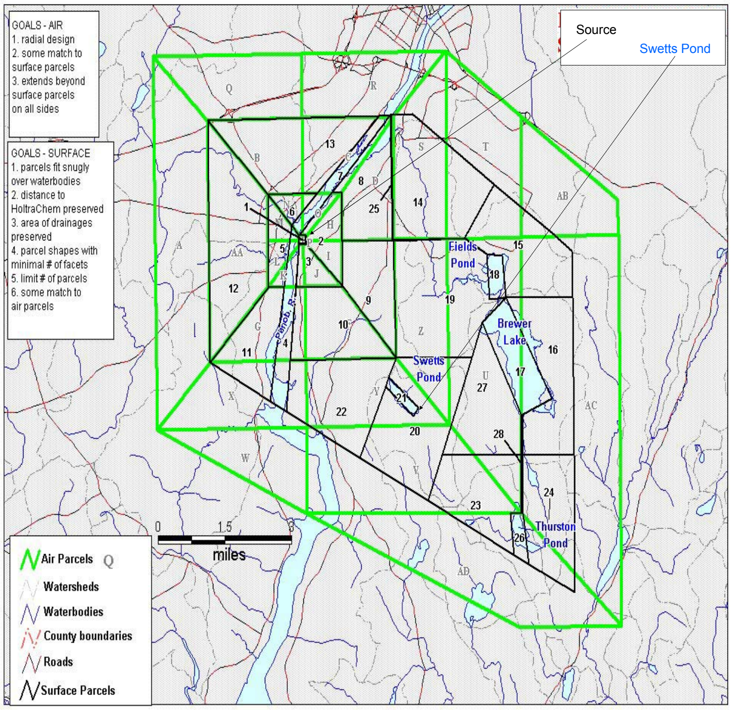


- **Parcels** are planar geographical areas used to subdivide the modeling region.
- **Volume elements** are bounded 3-dimensional spaces that define the location of one or more compartments.
- **Compartments** are spatial units within which it is assumed that chemical is homogeneously distributed.
  - **Abiotic** compartment types include, air, surface water, sediment, soil (surface, root zone , vadose zone), and ground water.
  - **Biotic** compartment types include several trophic groups of terrestrial and aquatic wildlife, such as birds, mammals, fish, terrestrial plants (leaf, root, stem), soil invertebrates, benthic invertebrates, algae and aquatic macrophytes. These trophic groups can be modeled relying on input values for representative species.

5. Case Study Description:

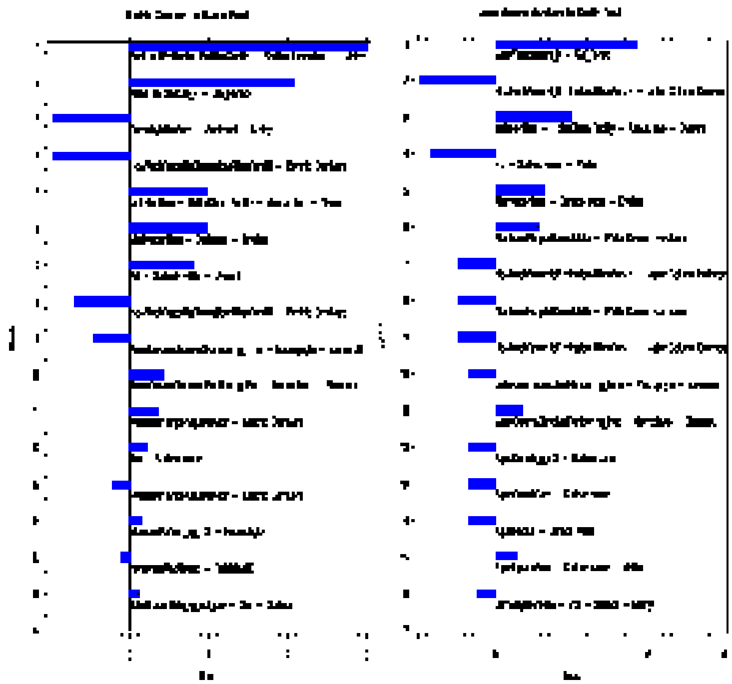
- **Simulation of Hg distribution (Hg0, Hg+2 & meHg) from air source in study area representative of rural NE U.S. w. several lakes and a river.**
- **Several simulations were performed which differed only as follows:**
  - **Steady-state solution with continuous point source of elemental & divalent Hg emissions.**
  - **Dynamic 30 year simulation with air boundary concentrations as only source of 2 Hg species.**
  - **Dynamic 30 year simulation including continuous point source of 2 Hg species, w/o boundary contributions.**
  - **Dynamic 30 year simulation including boundary concentrations, continuous point source, and initial media concentrations derived from 2nd simulation.**
- **All simulations used repeating 5 year met data set for nearby locations.**
- **For each simulation, results (mass, moles, concentration) were produced for all compartments in each volume element. The dynamic runs produced hourly results.**
- **Given the large amount of data produced, only particular aspects of the results are described here.**

6. Parcels, volume elements & compartments in Scenario



Volume Element	Compartments	Volume Element	Compartments
Air	Air	Surface Soil	Soil
			Leaf
Surface Water	Surface water		Leaf Particle
	Common Loon		Red-tailed hawk
	Mallard		Short-tailed Shrew
	Macrophyte		Raccoon
	Water Column Carnivore		Mouse
	Water Column Herbivore		Bald Eagle
	Water Column Omnivore		Mink
			Tree swallow
Sediment	Sediment		White-tailed Deer
	Benthic Invertebrate		Long-tailed Weasel
	Benthic Omnivore		Black-capped Chickadee
	Benthic Carnivore		Arthropod
Ground Water	Groundwater	Root Zone Soil	Soil
			Worm
Vadose Zone Soil	Soil		

9. Sensitivity scores – Parameters affecting methyl mercury concentration in top trophic fish in Swetts Pond



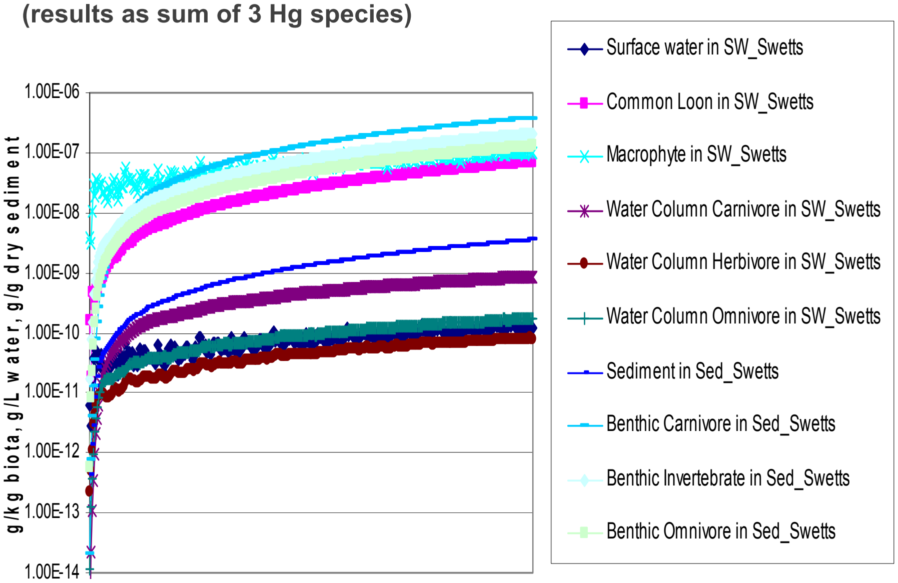
10. Dynamic, 30yr source only simulation results fall within reported measurement data.

- **Sediment**
  - Local measurements: 1e-7 – 3e-7 g/g, dry wt
  - Literature measurements: 7e-8 – 3e-7 g/g dry wt [U.S. lakes, USEPA 1997]
- **Surface water** (unfiltered)
  - Local measurements: 4e-9 – 2e-7 g/L
  - Literature measurements: 4e-11 – 7e-8 g/L [NJ lakes, USEPA 1997]
- **Fish**
  - Local measurements: 1e-4 – 1e-3 g/kg, wet wt*
  - Literature measurements: 3e-5 – 3e-4 g/kg wet wt [US freshwater, USEPA 1997]

*For comparison w. model results, fillet values were converted to whole body estimates by dividing by 2.

USEPA. 1997. Mercury Study, Report to Congress. Volume III: Fate and transport of mercury in the environment. EPA-452/R-97-005. RTP, NC.

7. Results – Dynamic 30 year simulation w. source (results as sum of 3 Hg species)



11. Next Steps

Complete Hg Case Study:
- Data analysis/interpretation of these runs
- Model Comparison w. 3MRA

Additional applications:
- PAHs,
- dioxins

12. Acknowledgements

Other TRIM.FaTE team members:

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