

Global Consumer Exposure Modeling Network - Sources/Transport & Fate Sub-Model Workshop Summary

European Commission - Joint Research Centre

Institute for Health and Consumer Protection Physical and
Chemical Exposure Unit

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Moderator



Definition of Sub-model

- Algorithm or relationship that exists at a very low or the lowest level in a larger, more comprehensive model predicting human exposure
- Output from the sub-model used as input to a more general model
e.g., Evaporative source rate => Estimate of Concentration (ventilation/dispersion => Estimate of exposure (human activity))



Workshop Participants

- **Arvanitis A.** JRC/IHCP/PCE (EU)
- **Bruinen de Bruin Y** JRC/IHCP/PCE (EU)
- **Delmaar C.** RIVM (Netherlands)
- **Flessner C.** EPA (USA)
- **Hanninen O.** KTL (Finland)
- **Hubal E.** EPA (USA)
- **Jantunen M.** KTL (Finland)
- **Jayjock M.** The Lifeline Group (USA)
- **Kephalopoulos S.** RC/IHCP/PCE (EU)
- **Koistinen K.** JRC/IHCP/PCE (EU)
- **Little J.** Virginia Polytechnic Inst. (USA)
- **Mason M.** EPA (USA)
- **Matoba Y.** Sumitomo (Japan)
- **McKone T.** University of California (USA)
- **Nazaroff W.** University of California (USA)
- **Pandian M.** Infoscience.com (USA)
- **Price P.** The Lifeline Group (USA)
- **Shade W.** Rohm and Haas, Co (USA)
- **Sheldon L.** EPA (USA)
- **Sutcliffe R.** Health Canada (CAN)
- **Won D.** National Research Council (CAN)
- **Wu K.** University of Taiwan (Taiwan)
- **Zhang Y.** Tsinghua University (China)



Presentations

- **McKone** (Berkeley) – Model uncertainty and evaluation of models
- **Matoba** (Sumitomo) – Microenvironment fugacity modeling
- **Pandian** (Infoscience.com)– How existing models handle sources and transport
- **Nazaroff** (Berkeley)– Intake fraction & reactive chemistry



Presentations

- **Little** (Virginia PolyTech) – Modeling VOC emissions from solids and liquids – theoretical constructs
- **Won** (CAN NRC) – Overview of Canadian National Research Council program on indoor sources – results and lessons learned
- **Jayjock** (The LifeLine Group) – Indoor transport models
- **Dalmaar** (RIVM) – RIVM aerosol studies and modeling



Developed a Complete Taxonomy of Sources

- **SOURCES of PARTICULATE Matter:**
 - Example: Handling “dusty” materials (aerosol).
- **VAPOR from DRY SOURCES:** Chemicals contained within, diffusing and emitting from solids
 - Example: Carpet and carpet backing
- **VAPOR from WET SOURCES :** Chemicals emitting from wet sources:
 - Example: Coatings (paint, varnish)
- **COMBUSTION SOURCES (PARTICULATE and VAPOR):** Example: wood burning
- **CHEMICAL REACTIONS :** example: reactions on surfaces



Workshop Consensus and Direction

- It was decided **not** to outline, characterize or explicitly build upon the currently available source sub-models beyond the draft workshop report done before the meeting
- Instead it was decided that we would consider building a framework for this body of scientific work from “the ground up”



Tiered Approach to Building Source Sub-Models from “the ground up”

- Emphasis on First Principle/Mechanistic Models
 - CHARACTERISTICS of Generic **wet source, dry source and particle source**
 - **ZERO TIER, FIRST TIER, N-TIER** (tiered approach to building mechanistic source models)
 - CHARACTERISTICS of Transport and Fate Models
 - **ZERO TIER, FIRST TIER, N-TIER** (tiered approach to building mechanistic T & F models)



Example: Generic wet sources

Zero tier—take all the mass and put it in air

First tier--simple dynamic mass-balance model (straight forward system)

Guo (1999) model

Mixture of active substances in wet material

Assume a film (~1mm) at constant concentration

Inputs needed

Vapor pressure (K_{aw})

External mass transfer coefficient

Second tier

Mixture of active substances in wet material

Vapor pressure (K_{aw})

More Complicated Mass transfer coefficient

Nth tier

Heterogeneous mixtures where one component alters the behavior of others

Able to handle substrate effects

Dynamic behavior of SVOCs affecting emissions.

Transition from wet to dry

Time and location dependent diffusivity

Exogenous reactive chemistry

Endogenous (incidental/intentional) reactive chemistry



Work Products

- Identification of existing source sub-models – draft report and references
- Defined a Taxonomy of Sources
- Identified the attributes and characteristics of First Principle Mechanistic Source and Transport/Fate models to be used in a tiered approach to exposure/risk assessment.

