Rapid Assessment of Exposures and Doses to Atmospheric Contaminants using the Pre-Computed Modeling Approach

Sastry S. Isukapalli and Panos G. Georgopoulos • Computational Chemodynamics Laboratory (www.ccl.rutgers.edu)
Environmental and Occupational Health Sciences Institute, a Joint Institute of UMDNJ-Robert Wood Johnson Medical School and Rutgers University, Piscataway, NJ

Summary

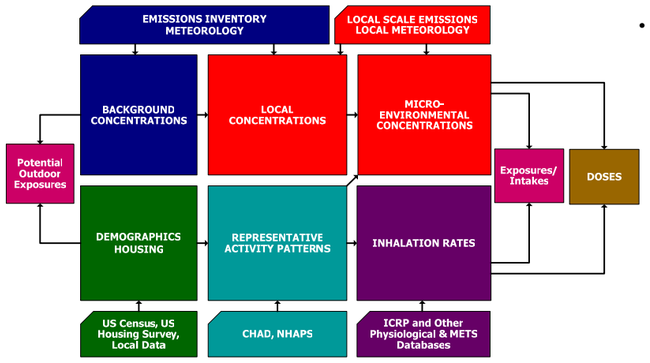
Context:
- Population-based exposure assessment is computationally demanding
  - several number of steps involved
  - large number of sampled population required to obtain statistically representative results
  - requires weeks (after obtaining ambient calculations), to months (including ambient air quality calculations) on a single machine

Need:
- Techniques to improve computational efficiency, without compromising on the accuracy of the results
- A system that can facilitate quick sensitivity testing of the exposure assessment process

Traditional Approaches:
- Simple models (may lead to over-simplification)
- Approximation of models (may require large number of model runs, and still produce a coarse approximation)
- Clustered computers (expensive; disk/network sharing bottlenecks)

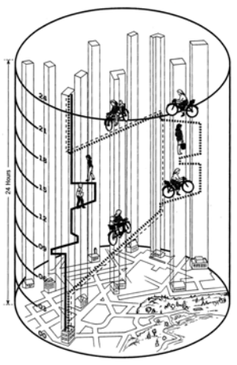
Proposed Approach:
- The pre-computed modeling approach provides a fast alternative
  - results identical to running the full model
  - can be synchronized with the full model
  - amenable to iterative refinement

Steps in Exposure Assessment using MENTOR/SHEDS-1A



Summary of steps in exposure assessment using MENTOR/SHEDS-1A [Modeling ENvironment for TOtal Risk studies (MENTOR) using the Stochastic Human Exposure and Dose Simulation (SHEDS) approach in a "One Atmosphere" (1A) setting] (Georgopoulos et al. 2005).

Rationale for Population-Based Exposure Assessment



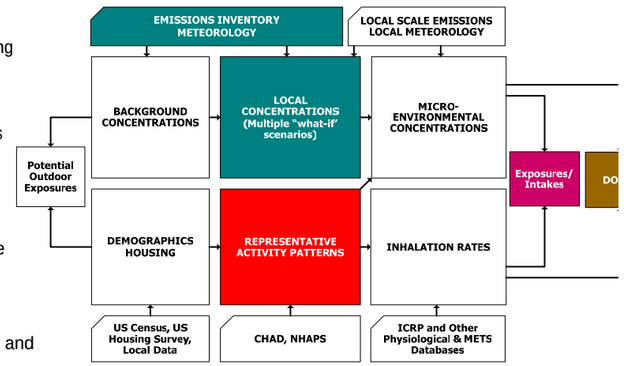
People/Time/Space:
Adapted from Parkes & Thrift (1980)

Exposures and doses for one person
- Physiological characteristics (age, gender, body weight, etc.)
- Microenvironmental factors (ventilation rate, house size, etc.)
- Activity patterns (exercise, sleep, commuting, etc.)
- Location of microenvironment (school, store, home, car, etc.)
- Local ambient concentrations

Exposures and doses for population
- Physiological characteristics (age, gender, body weight, etc.)
- Microenvironmental factors (ventilation rate, house size, etc.)
- Activity patterns (exercise, sleep, commuting, etc.)

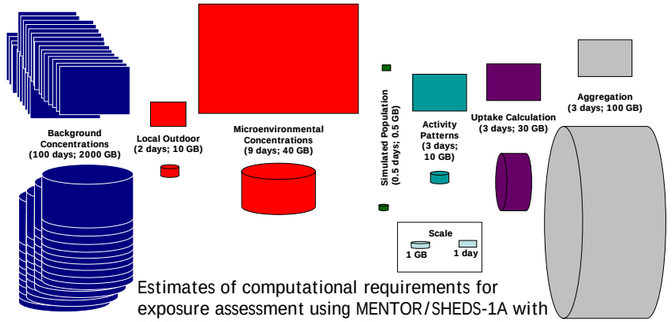
Relevant Databases
- Census Database from US Census Bureau
- US Housing Survey
- Databases of representative activity patterns (e.g. the Consolidated Human Activity Database, CHAD, McCurdy 2000)
- Emergency response strategies (e.g. evacuation/shelter-in-place)

Motivation for Pre-Computed Modeling

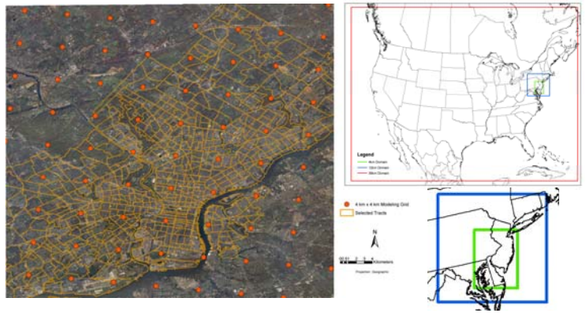


Pre-computed modeling enables performing multiple model runs with a major subset of options staying constant, and is applicable for:
- "What-if" scenarios for sensitivity testing
  - quickly assess the impact in changes in concentrations on exposures/doses (e.g. 10% increase/reduction, etc.)
  - avoid variability introduced in multiple exposure simulations
- Supporting emergency event response
  - Data base of "pre-computed runs" for multiple response strategies (e.g. evacuation/shelter in place)
  - quickly assess appropriate response strategy

Computational Requirements for Exposure Assessment

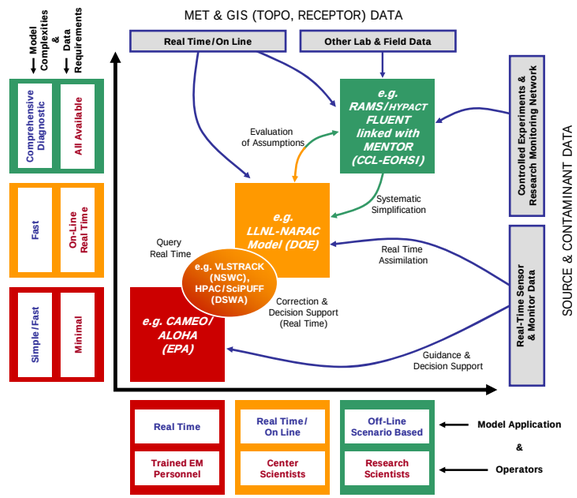


Estimates of computational requirements for exposure assessment using MENTOR/SHEDS-1A with CMAQ. Performing multiple "sensitivity tests" is computationally infeasible for many organizations.



The estimates of computer requirements shown above are based on MENTOR/SHEDS-1A simulation for the urban Philadelphia/Camden region shown here. Background concentrations were obtained from the CMAQ (Community Multiscale Air Quality) model run with the toxics version of SAPRC99 chemical mechanism – results from the 4 km x 4 km were used.

Emergency Events Models for Atmospheric Releases



A set of emergency event models classified based on model detail and computational requirements. The aim of this work is to facilitate use of detailed models quickly by first responders.

Mathematical Formulation

"Microenvironmental factors" based calculations

$$C_{microenvironmental} = F_{additive} + F_{penetration} \cdot F_{proximity} \cdot C_{ambient}$$

$$C_{F,microenvironmental} = F_{penetration} \cdot F_{proximity}$$
$$C_{A,microenvironmental} = F_{additive}$$

Perform calculations for each: activity m, day n, individual i, census tract j

$$C_{residential} = \frac{P \cdot A}{A + k} C_{ambient}$$

or

$$C_{residential} = \frac{P \cdot A}{A + k} C_{ambient} + \frac{S_{indoor}}{(A + k) \cdot V \cdot T}$$

$$C_{F,residential} = \frac{P \cdot A}{A + k}$$
$$C_{A,residential} = \frac{S_{indoor}}{(A + k) \cdot V \cdot T}$$

Subsequent model runs:

$$C_{exposure;i,j,m,n} = C_{A;i,j,m,n} + C_{F;i,j,m,n} \cdot C_{ambient;(j,\, t_{activity;m,n})}$$

Pre-computed tables for intakes/doses

$$R_{ventilation} = BMR \cdot METS \cdot EETOVO2 \cdot VQ$$
$$D = C_{exposure} \cdot \Delta T \cdot R_{ventilation} = (C_A + C_F \cdot C_{ambient}) \cdot \Delta T \cdot R_{ventilation}$$
$$D_F = C_F \cdot \Delta T \cdot R_{ventilation}$$
$$D_A = C_A \cdot \Delta T \cdot R_{ventilation}$$

Dose for individual i in census tract j on day m

$$D_{i,j,m} = \sum_{n=1}^{N_{activities;i,j,m}} \left(D_A(i,j,m,n) + D_F(i,j,m,n) \cdot C_{ambient;(j,\, t_{activity;i,j,m,n})} \right)$$

Perform calculations for all individuals in all census tracts to obtain population estimates

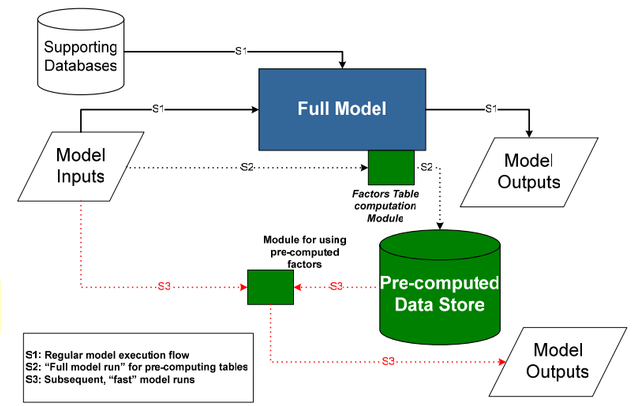
Reduction of Computational Time using Pre-Computed Modeling Blocks

Goals:
- Results must be identical to the original model
- Pre-Computed model must be synchronized with the original model
  - should be amenable to iterative refinement

Approach:
- Develop piece-wise (event-wise) linear relationships for each activity/exposure event
  - Different from "a linear factor approach"
- Approach readily extensible to complex, nonlinear relationships

Tradeoff:
- Disk space for storing multiple "pre-computed" modules
- Planning for scenario developments (e.g. for emergency response)
- Analogous to tables of endgame strategies in chess
- Full model has to be run for each scenario

Overview of the Pre-Computed Modeling Architecture



Discussion

- Conceptual development of the pre-computed modeling framework completed
- A prototype of the system used in conjunction with MENTOR/SHEDS-1A
- System reproduced identical results as full model simulation
- Execution time reduced from several days to under an hour
- Storage space for the pre-computed factors is about two orders of magnitude as the full model
- A scientist can quickly download the factors and perform preliminary analyses
  - without having to understand all the complexities in the models
  - without having to download large datasets
- Provides a means for fast assessment of exposures and risks
- Potential use for rapid sensitivity analyses
- However, the full model has to be run "at least once"
- Applicable only for the given "scenario" (e.g. set of census tracts)

Acknowledgements

Base Funding for the Ozone Research Center is Provided by the State of New Jersey Department of Environmental Protection. The work presented here has been funded by a University Partnership Agreement (UPA) between the USEPA and EOHSI (Cooperative Agreement #831625).