Homeland Security Research at the EOHSI Center for Exposure and Risk Modeling (CERM)

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Computational Chemodynamics Laboratory
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Overview of Homeland Security Research at CERM

Aims:

• to develop, evaluate and refine computational tools for characterizing population exposures and doses associated with chemical and biological agents released during emergency events

Computational tools:

• predictive environmental and biological models for contaminant release, transport, and fate
  - multiple spatial scales (e.g. regional, urban, local, neighborhood, microenvironmental, personal, organ/tissue)
  - multiple temporal scales (e.g. from seconds to weeks)

• integrated exposure information systems for dynamic linking of models with comprehensive databases and Geographic Information Systems characterizing
  - environments/microenvironments (via e.g. meteorology, hydrogeology, land use and cover, building properties, etc.)
  - populations (via demographic attributes, activity patterns, etc.).
Examples of Currently On-Going Homeland Security Related Projects at CERM Include:

- Evaluation of existing environmental fate/transport models for their applicability and limitations in emergency situations; refinement of models
- Modeling studies of emergency events (such as fires) at or near nuclear and hazardous waste facilities
- Development of prototype source-to-dose modeling systems for characterizing multipathway exposures to chemical and biological warfare agents
- Reconstruction of population exposures to the contaminants released from the fires and collapse of the World Trade Center on 9/11/2001 to provide analyses of lessons learned and to support a variety of health impact studies
- Development and application of computationally efficient “model/data fusion” techniques for real-time
  - inverse problem solution (source characterization)
  - Bayesian real-time model “calibration”
  - uncertainty characterization and reduction
- Analysis and optimization of spatiotemporal contaminant monitoring network designs.
- Development of protocols for hospital personnel response to emergency events involving chemical warfare agents
Modeling for Emergency Response: A Framework for Model/Data Fusion with Application to Both Forward and Inverse Problems

MONITORS

SOURCE

SENSITIVE RECEPTORS

EXPOSURE & RISK ANALYSIS

1ST Level Transport Problem

Inverse Problem

Bayesian Model/Data Fusion

2ND Level Transport Problem

Inverse Problem

Homeland Security Research at CERM

Computational Chemodynamics Laboratory - EOHSI
Interlude: Example EPANET Application for Distribution of a Toxican in Municipal Water Network Involving Two Suppliers
Contaminant Dispersion Models Linked With GIS-Based Information on Monitors and Receptors

MET & GIS (TOPO, RECEPTOR) DATA

- Real Time/On Line
- Other Lab & Field Data

Response Center Modeling

- “Field Model” (on Wireless Laptop or PDA)
- Real Time
- Real Time/On Line
- Off-Line Scenario Based

- Real Time Senor & Monitor Data
- Controlled Experiments & Research Monitoring Network

Research Lab Modeling Prognostic/Diagnostic

- Evaluation of Assumptions
- Systematic Simplification

- Correction & Decision Support (Real Time)
- Real Time Assimilation

- Guidance & Decision Support

Model Application & Operators

- Trained EM Personnel
- Research Scientists
- Research Scientists
- Center Scientists
Example Ia – Regional Scale: Trajectory Analysis for Screening Regional Scale Characterization Using the NOAA HYSPLIT Model (Potential for Long Range Transport of the WTC Plume)
Example Ib - Mesoscale: Instantaneous Views of the WTC Plume, Simulated Using the RAMS/ HYPACT Prognostic System

Top: 3-d Plume View; Bottom: Surface Layer Wind Fields and Concentration Gradients (Concentration Fields are Normalized with Respect to Maximum of Each Instance)
Understanding Limitations and Refining Models for Environmental Releases - Example II: Calculations of Hypothetical Release in NJ using the ALOHA Model

Legend
- NJ_Schools
- Chemical Release Model
  - Uncertainty Region
  - Above LOC Region
- NJ_Hospitals
- Zip Code Areas
- Census Tracts
- Urban Areas
- Parks

July 12, 1995, 2:00 pm

July 12, 1995, 7:00 pm
Simulation of the Same Case Study With a Comprehensive System that Accounts for Sea Breezes (RAMS-HYPACT) Produces a Very Different Picture of the Dispersing Plume

\[ z = 125.0 \text{ m} \quad t = 2000 \text{ GMT} \]

\[ v = 87.30 \text{ km} \quad t = 2340 \text{ GMT} \]
Example II: Hypothetical Anthrax Release Simulation Results from CALPUFF - Model Setup Critically Affects Predictions

Instantaneous release modeled with CALPUFF at 1km resolution (08:00, 12:00 & 16:00)

Instantaneous release modeled with CALPUFF at 250m resolution (08:00, 12:00 & 16:00)
Example III: EIS for the Savannah River Site Incorporates a Variety of Spatial/Temporal Databases
3-D Views of Smoke Plume from Controlled Forest Fire in the Vicinity of SRS (Superimposed to the ABL Wind Field)

- the smoke plume at 2200 GMT (5:00 PM local time)
- the smoke plume at 0800 GMT (3:00 AM local time, next day)
Caveat: Neighborhood Scale Effects Can Modify Significantly Estimates from Atmospheric Transport Models or from Monitor Interpolations (Barriers, Channeling, Local Flows, Trapping): Need for Both CFD & Simplified Models
Fact: In addition to time and geographic location, factors such as dynamic microenvironmental attributes, demographic and physiological characteristics, activity patterns, etc. differentiate significantly the exposures and doses of individuals (and of selected subpopulations) that result from an environmental (emergency) event.

Challenge: All relevant information must be integrated in a consistent/unifying framework (Spatiotemporal Exposure Information System).

Example: Dependence of inhaled fine PM dose on gender, age, and activity (MET = Metabolic Equivalent of Tasks).
Integrated Framework for Reconstructing Exposures to the WTC Plume

1. "Baseline Definition": Estimate background levels of air pollutants at various scales through:
   a. multivariate spatiotemporal analysis of monitor data (STRF, BME)
   b. emissions-based multiscale air quality modeling

2. Estimate spatiotemporal levels of outdoor contamination at neighborhood scale (e.g. for census tracts, or local grid) via:
   a. "constrained" analysis of monitor data
   b. application of multiscale model at high resolution
   c. physical "corrections" of the estimates of multiscale fate and transport model

3. Estimate pollutant “profiles” in microenvironments through:
   a. regression of observational data
   b. simple mass balances
   c. gas/aerosol dynamics modeling
   d. CFD & transformation modeling

4. Characterize attributes of populations (geographic density, age, gender, race, income, etc.):
   a. select fixed-size sample populations that statistically reproduce essential demographics, or
   b. divide population of interest into exhaustive set of cohorts

5. Develop activity event (or exposure event) sequences for each member of the sample population, or for each cohort, from:
   a. existing databases from composites of past studies (for baseline assessment)
   b. study-specific information (special registries)

6. Calculate appropriate inhalation (and other relevant uptake*) rates for the members of the sample population combining:
   a. physiological attributes of the study subjects and
   b. activities pursued during the individual exposure events
   *e.g. non-dietary ingestion

7. Combine intake rates and microenvironmental concentrations for each activity event to assess exposures

Emissions: NEI (NET, NTI), State; Processing with SMOKE, EMS-HAP, MOBILE, NONROAD, FAAED, BEIS, etc.; Air Quality: AIRS, NADN; Land Use/Land Cover: NLDC; Elevation: NED
Meteorology: NWS, NCDC; Modeling: HYSPLIT, MM5, RAMS, CALMET, CALPUFF, HYPACT, CMAQ

US Census, US Housing Survey, Local Data (e.g. Lotlnfo, NYC BaseMap)
Baseline: CHAD, NHAPS; Event-Specific: Special Registries
ICRP and Other Physiological & METS Databases

WTC Site-Specific Emissions Modeling; Local and Mesoscale Transport and Fate Modeling: FLUENT, RAMS
MENTOR/SHEDS baseline simulation, for 11/19/2001, of inhaled doses of PM2.5 due to outdoor and indoor sources for the population in census tracts within 2.5km of WTC.
CCL Research on Environmental Contaminant Release, Transport/ Fate, and Exposure/ Dose for Emergency Events

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