

*DOE Operational User Requirements and Dispersion  
Modeling Capabilities*

*DOE Chemical & Biological Nonproliferation Program:  
Modeling and Prediction*

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Department of Energy (DOE)*

Workshop on  
Multi-scale Atmospheric Dispersion Modeling  
within the Federal Community

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## DOE Dispersion Modeling Operational Activities

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- Facility Safety Analysis
  - Determine potential consequences of a facility before construction or modification; use during operation for risk assessment
- Facility Emergency Preparedness and Response
  - Develop hazard assessments, emergency action levels, and modeling systems to use in emergency response
- Deployable Assets for Emergency Response (ARG, FRMAC, NEST, JTOT)
  - Resources to protect public from major radiological accidents and terrorist events
- Facility Annual Environmental Reporting
  - Document exposure to public from routine operations

## DOE Dispersion Modeling Operational Activities

Activity - Description	Authority or Requirement	Guidance	Dispersion Modeling Approach
Facility Safety Analysis	DCE Order 5480.23 (1997), NRC NUREG-1320 (1988) & CR-6410 (1998)	DOE-STD-1027-92 & 3009-94, DOE-HDBK-3010-94, NRC Reg. Guide 1.145 (1983), Accident Analysis Guidebook (2000), Accident Phenomenology & Consequence (APAC) Working Group Reports (1997-2000)	Graded approach – Model complexity commensurate with complexity or scale of effect, i.e., simple Gaussian to complex 3-D numerical codes
Facility Emergency Preparedness & Response	DCE Order 151.1 (1997, currently under revision)	DCE Guide 151.1 (1997, currently under revision), DOE Modeling Resources (1995)	Graded approach – Model complexity commensurate with complexity or scale of effect, i.e., simple Gaussian to complex 3-D numerical codes
Deployable Assets for Emergency Response (ARG, FRMAC, NEST, JTOT)	Federal Response Plan (FRP, 1995), Presidential Decision Directive 39 (PDD 39, 1995)	Federal Radiological Emergency Response Plan (FRERP, 1996), Overview of FRMAC Operations (2000), DoD Nuclear Weapons Accident Response Procedures (NARP, 1995)	Graded approach – Deployed teams use local models in the field and reach back to NARAC models
Facility Annual Environmental Reporting	DCE Orders 5400.1 & 231.1, CERCLA, SARA Title III, Nat'l. Emission Stds. for Haz. Air Pollutants (NESHAPS) 40 CFR 61	EPA Model Guideline	EPA annual model

## DOE Dispersion Models Used Within DOE

Activity	Technical Forums	Dispersion Models Used																																
Facility Safety Analysis	DCE Energy Facility Contractors Group Safety Analysis Working Group (EFCOG SAWG) www.sawg2000.org	<table><tr><td>Radiological models:</td><td>GXQ</td><td>Chemical models:</td><td></td></tr><tr><td>AI-RISK</td><td>HOTSPOT</td><td>ADAM</td><td>HGSystem</td></tr><tr><td>AXAIR89Q</td><td>MACCS2</td><td>ALOHA</td><td>INPUFF</td></tr><tr><td>BNLGP</td><td>MATHEW/ADPIC</td><td>CALPUFF</td><td>SLAB</td></tr><tr><td>COSYMA</td><td>PAVAN</td><td>CASRAM</td><td>SCIPUFF</td></tr><tr><td>ERAD</td><td>PSAC 5</td><td>FEM3</td><td>TSCREEN</td></tr><tr><td>ETMOD</td><td>TRAC PA/HA</td><td></td><td></td></tr><tr><td>GENII</td><td>UFOTRI</td><td></td><td></td></tr></table>	Radiological models:	GXQ	Chemical models:		AI-RISK	HOTSPOT	ADAM	HGSystem	AXAIR89Q	MACCS2	ALOHA	INPUFF	BNLGP	MATHEW/ADPIC	CALPUFF	SLAB	COSYMA	PAVAN	CASRAM	SCIPUFF	ERAD	PSAC 5	FEM3	TSCREEN	ETMOD	TRAC PA/HA			GENII	UFOTRI		
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Facility Emergency Preparedness & Response	DCE Emergency Management Issues Special Interest Group (EMI SIG) http://www.orau.gov/emi/  DCE Subcommittee on Consequence Assessment and Protective Actions (SCAPA) http://www.scapa.bnl.gov/	ALOHA (NOAA; National Safety Council) CAPARS (Hodgin, AlphaTrac) Epicode (Homann Associates) ERAD (Boughton, Sandia Natl Lab) HOTSPOT (Homann, LLNL) MDIF-VIS (NOAA ARL, INEEL) MIDAS (PLG) NARAC - ADAPT/LODI (Sugiyama & Nasstrom, LLNL) PGEMS (Allwine, PNNL) WINDS (Savannah River Lab)																																
Deployable Assets for Emergency Response (ARG, FRMAC, NEST, JTOT)	ARG, FRMAC, NEST, JTOT Working Groups http://www.dp.doe.gov/emergencyresponse/ http://www.nv.doe.gov/programs/frmac/	Local models used in the field: HOTSPOT, ERAD Reach back to NARAC models: ADAPT/LODI																																
Facility Annual Environmental Reporting	EPA SCRAM & Modeling Conferences http://www.epa.gov/scram001/	CAP-88																																

# **DOE Dispersion Modeling Capabilities Graded Approach**

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## **Hotspot Health Physics Codes**

Deployed to emergency response personnel

## **SNL Atmospheric Dispersion and Consequence Prediction Capability**

Deployed with expert atmospheric dispersion scientist

## **LLNL National Atmospheric Release Advisory Center (NARAC)**

Reach-back to national center with expert assessment staff

## Hotspot Health Physics Codes

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- **Purpose**

- To provide emergency response personnel and emergency planners with a fast, field-portable set of software tools for evaluating incidents involving radioactive material.

- **Applications**

- Estimate the radiological impact following the release of radiological material from a continuous or puff release, explosive release, fuel fire or an area contamination event.

- **Dispersion Model**

- A Gaussian plume/puff model with virtual source terms to model the initial atmospheric distribution of source material.

- **Health Effects**

- Dose conversion factor library for inhalation, submersion and ground shine (ICRP-30 Library).

## **SNL Atmospheric Dispersion and Consequence Prediction Capability**

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- **Purpose**

- **Provide, on a field deployable system, predictions of the near field consequences which result from the dispersion of nuclear, chemical and biological releases**

- **Applications**

- **Response to WMD terrorism incidents**
- **Threat and safety analyses**
- **Probabilistic risk assessments**
- **Environmental impact statements**



## Steps in Prediction Process

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- **Characterize Source Term (Amount, Particle Size Distribution, Agent Viability, etc.) as a Function of Release Type**
  - Explosive
  - Non-explosive aerosol
  - Fire-driven
  - Aerial
  
- **Model Atmospheric Transport and Diffusion**
  
- **Estimate Dose and Health Effects**
  - Toxicological models available for full range of chemical and biological agents and over 800 radionuclides



## **Steps in Prediction Process (cont'd)**

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- **Develop Mitigation Strategy**
- **Communicate Results in a Format More Directly Useful to Decision Makers**
  - **Model predictions translated into health impacts**
  - **Results presented in an hierarchical format**
    - **Key results presented first**
    - **Additional details and supporting information available as needed**
  - **Non-expert able to “read” essential results quickly and unambiguously**
  - **Results for both unmitigated and mitigated release**

## **AIRRAD Radionuclide Fallout Model**

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- **Model Description**

- Implements methodology of DNA SIMFIC model
- Square-root-of-time relationship for buoyant rise
- Gaussian puff approach for turbulent dispersion
- Workstation or PC compute platform

- **Capabilities**

- Large number of hazard indicators
- Graphical user interface
- Full integration of model predictions with worldwide GIS

## **ERAD High Explosive Dispersal Model**

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### **■ Model Description**

- **Integral technique for source buoyancy**
- **Probabilistic approach for turbulent dispersion**
- **Parameterization of planetary boundary layer based on contemporary scaling theory**
- **Workstation or PC compute platform**

### **■ Capabilities**

- **Gaseous and particle sources**
- **Treats penetration of elevated inversions**
- **Graphical user interface**
- **Full integration of model predictions with worldwide GIS**

## National Atmospheric Release Advisory Center

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- NARAC's *mission* is to provide timely and credible assessment advisories to emergency managers for nuclear and other hazard releases to the atmosphere and thereby minimize the exposure of the population at risk.
- The mission requirements apply worldwide wherever and whenever DOE and DoD Emergency Planning and Response programs have a requirement or our government deems there is an event of interest.

# National Atmospheric Release Advisory Center (NARAC)

*Real-time advisories for hazardous atmospheric releases*

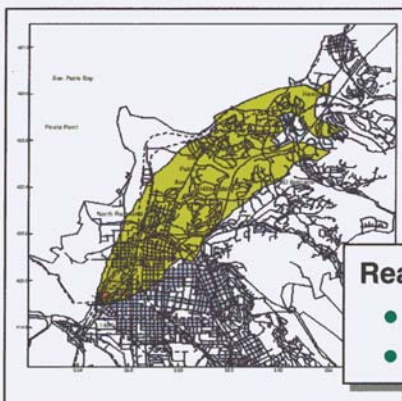
## World-wide coverage

- Terrain & land-surface
- Vector & raster maps
- Real-time weather data



## National Center at LLNL

- Expert assessment staff
- Advanced modeling system



## Real-time Hazard Advisories

- Available within minutes
- Distributed electronically

NARAC staff operates the center, trains users and deploys for special events

# **Access to the National Atmospheric Release Advisory Center (NARAC)**

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**National Center in Livermore**



**Dedicated Intranet  
or Dial-up**

**Communication links using  
Internet protocols (Internet  
intranet, dial-up, wireless)**

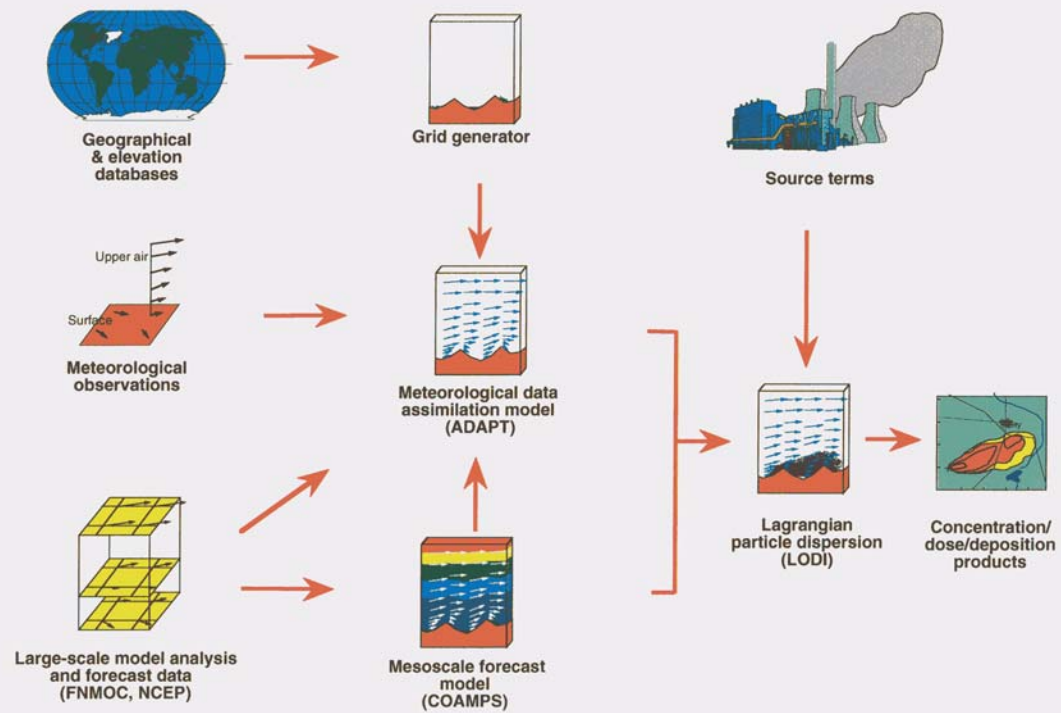


**Site Workstation System (SWS)  
at DOE/DoD Facilities**



**Internet Remote Access (IRA) System  
for Local EOC or  
Deployment to Remote Site  
(Under Development)**

# NARAC Modeling System





## NARAC Weather Forecast Model (COAMPS)

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- **COAMPS** - Naval Research Laboratory model (Hodur, 1996)
- **Grids**
  - Arakawa-C grid, continuous terrain representation, vertical coordinate
  - Multiple nested grids
- **Data analysis and initialization**
  - Multivariate optimum interpolation analysis of winds and temperature
  - Time-dependent boundary conditions (Davies, QJRM 1976; Perkey and Krietzberg, MWR 1976)
- **Dynamics**
  - Non-hydrostatic compressible (Klemp and Wilhelmson, JAS 1978)
  - 2<sup>nd</sup> order advection, 4<sup>th</sup> order diffusion
- **Atmospheric physics**
  - Radiation (Harshvardhan, JGR 1987)
  - Explicit moist physics (Rutledge and Hobbs, JAS 1983)
  - Convective precipitation physics (Kain and Fritsch, JAS 1990; Kuo, JAS 1979)
  - Boundary layer physics (Mellor and Yamada, 1982)
  - Surface layer physics (Louis, 1979)

## NARAC Meteorological Data Assimilation Model (ADAPT)

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- **Grids**
  - Variable-resolution grids
  - Continuous terrain representation,  $\sigma_z$  vertical coordinate
  - Map projection for multiple scales
- **Assimilation of meteorological and land-surface data**
  - Observational data (e.g, surface, tower, profiler, rawinsonde)
  - Weather forecast model data (e.g, AVN, COAMPS, NOGAPS, ETA)
  - Land-surface data (e.g,  $z_0$ ,  $d$ , land use category)
- **Interpolation and parameterization**
  - Multiple interpolation algorithms
  - Vertical parameterization options
- **Meteorological variables**
  - Non-divergent wind field ( $\nabla \cdot V = 0$ ) based on variational principal and finite-element spatial discretization and conjugate gradient solution method
  - Temperature, pressure, humidity, and other scalar fields
  - Precipitation
  - Diagnostic eddy diffusivity parameterization based on scaling relationships
  - Turbulence scaling parameters derived from land-surface and surface meteorological data

## **NARAC Dispersion Model (LODI)**

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- Lagrangian stochastic (Monte Carlo) diffusion method
- Nested meteorological data grids
- Variable-resolution concentration and deposition grids
- Multiple, moving receptors
- Point, line, area, and Gaussian sources
- Aerosol mass-size distributions (log-normal or table)
- Multiple, moving, time-varying sources
- Momentum and buoyancy plume rise
- Decay and production of radionuclides in decay chains
- First-order decay of biological and chemical material
- Dry deposition (from gravitational settling velocity and deposition resistance)
- Precipitation scavenging (from aerosol size and precipitation rate)

## NARAC Model Testing and Evaluation

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- **Model evaluation**
  - Testing of individual models
  - Comparisons with known analytic solutions
  - Component testing of individual physical processes and numerics
- **Laboratory experiments**
  - Comparisons with wind/water tank experimental results
- **Field experiment case studies (ADAPT/LODI)**
  - Project Prairie Grass: Flat terrain; continuous near-surface point source of  $\text{SO}_2$ ; 50-800 meter downwind distance
  - Savannah River Mesoscale Atmospheric Tracer Studies (MATS) : Rolling, tree-covered terrain; 15-min  $\text{SF}_6$  release at 61 meters; 30 km range
  - Diablo Canyon Tracer Study (DOPPTX) : Hilly, coastal terrain; continuous and pulsating  $\text{SF}_6$  releases at surface and 71m; 1-40 km range
  - European Tracer Experiment (ETEX) : Continental Europe, and U.K; 12-hr continuous perfluorocarbon tracer gas release near surface; 20-2000 km
- **Operational testing**
  - Performance and speed
  - Robustness
  - Default model input settings

## DOE - DTRA (DoD) Model Intercomparison Project

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### ➤ Purpose

- Collaborative effort to advance the atmospheric hazard assessment prediction capabilities of both the DOE and DoD through a scientifically based joint modeling system evaluation and comparison study

### ➤ Plan

- Develop a joint understanding of the DOE and DoD modeling systems
- Evaluate the modeling systems for an initial set of experimental data sets and a variety of conditions (meteorology, land-surface, turbulence, source)
- Distinguish variations due to model physics and numerics from differences due to operational default choices

### ➤ Comparison Metrics

- Statistical criteria: spatially/temporally paired point-to-point statistical comparisons of model output and measured concentration values (ratio factors, normalized mean square error, bias, etc.)
- Graphical criteria: overlays of measured values and model contours

### ➤ Initial Case Studies (FY00)

- Dispersion model-to-model comparisons for simple scenarios
- Project Prairie Grass (microscale experiment, 1956)
- Dugway Phase 1 (DoD microscale puff dispersion experiment, 1996)



**DOE CBNP**  
**Modeling and Prediction**

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**Chem-Bio Transport and Fate  
in Urban Environments**

Argonne National Laboratory  
Lawrence Berkeley National Laboratory  
Lawrence Livermore National Laboratory  
Los Alamos National Laboratory  
Pacific Northwest National Laboratory  
Sandia National Laboratories

Department of Energy  
Chemical & Biological Nonproliferation Program

# Goal

## Modeling and Prediction

**Building Interiors**



**Subway**



**“...to accurately predict the dispersion and ultimate fate of chemical and biological agents released into the urban environment...”**

**Multiple Interacting Scales**

**Urban-Regional**



**Exterior Building**



Counterterrorism Incident Response in  
Urban Areas and at Special Events



## Multi-Scale Transport Models

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- **COMIS Multizone Building Interiors Model**
- **STAR-CD Building Interior CFD Model**
- **SES Subway System Model**
- **FEM3CB Exterior Building Scale CFD Model**
- **HIGRAD Exterior Many Building CFD Model**
- **COAMPS/LODI Exterior Parameterized Urban-Regional Model**

## **Building Scale Airflow and Dispersion Model (FEM3CB)**

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- **Computational Fluid Dynamics (CFD) code based on the finite element approach**
- **Flexible grid system capability including variable resolution, distorted meshes and explicit representation of terrain**
- **Capability of resolving individual buildings in great detail or few buildings at varying resolutions**
- **Runs on ASCI's massively parallel platforms**
- **Current model physics:**
  - **Neutral or heavier-than-air (chemical) agents**
  - **Aerosol physics (biological agents)**
  - **Surface heating and shading**
  - **Tree canopy parameterization**
  - **Reynolds-averaged (RANS) and Large Eddy Simulation (LES) turbulence models**
  - **First order UV degradation submodel**

# Salt Lake City

## Fall 2000 Field Experiments

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- **Single Building (SF6) [CBNP]**
  - 2 to 4 hour experiments
  - Instantaneous line source outside building (>1 ppm SF6)
  - 45 Tracer samplers located inside and outside building (15 bags-programmable)
  - 5 to 10 minute sampling times in bags
  - 6 Fast-response SF6 instruments (1 Hz data)
  - 6 Sonic anemometers (10 Hz data)
  - 1 Open-path FTIR for SF6 mapping
- **Multi-Building to Urban-Scale (SF6-PFT) [CBNP/VTMX]**
  - 12 to 18 hour experiments
  - 1 2 to 3 hour PFT point release at single building
  - 1 6 to 8 hour PFT point release downtown
  - 40 Tracer samplers (12 bags/CATS tubes-programmable)
  - 15 minute to 1 hour sampling in bags/CATS
  - 24 Temperatures loggers for urban temperature mapping
  - 3 Surface weather stations
- **Urban-Scale to Mesoscale (PFT) [VTMX]**
  - 12 to 18 hour experiments
  - 2 6 to 8 hour PFT point releases outside of downtown
  - 60 PFT samplers (23 tubes-programmable)
  - 1 to 3 hour PFT sampling in tubes
  - 6 Radar profilers (with RASS)
  - 4 Sodars
  - 3 Tethersonde systems
  - 1 Doppler lidar
  - 3 Rawinsonde systems
  - 6 3-D sonics for fluxes
  - 10 Surface weather stations
  - NWS rawinsondes