

Atmospheric Dispersion Modeling: Recent Advances and Future Needs

NAS/BASC Panel: Frontiers and Challenges in Atmospheric Dispersion Modeling

December 3, 2014

Gayle Sugiyama, Ph.D.



National Atmospheric Release Advisory Center

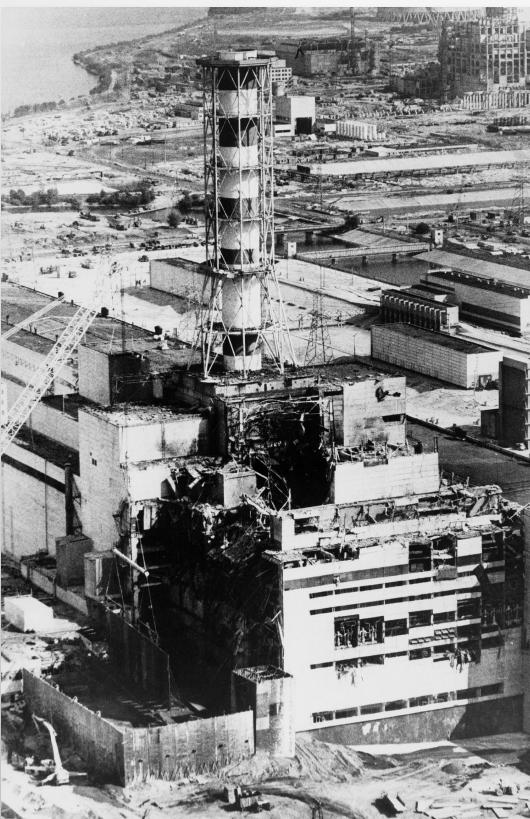
NARAC

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC. The Department of Homeland Security sponsored part of the production of this material.

LLNL-PRES-664995



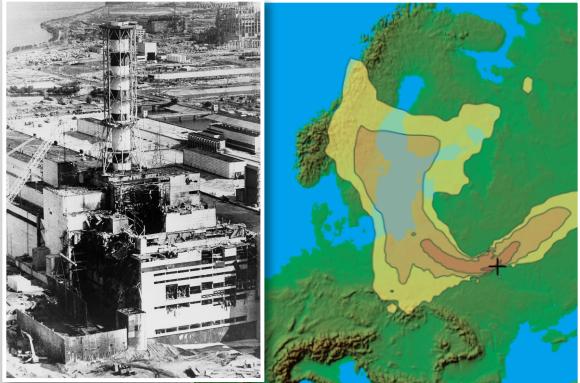
NARAC Provides Critical Information to Protect the Public and the Environment



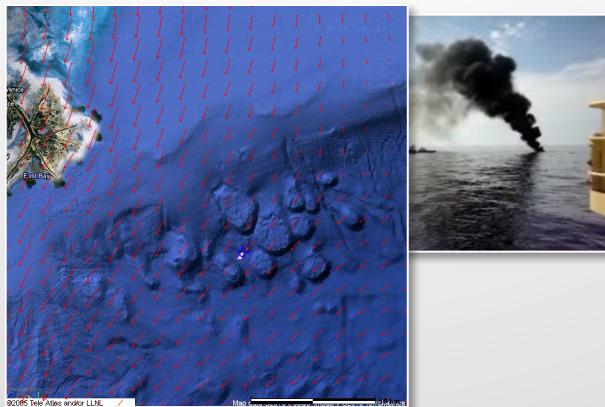
Hazardous airborne releases are a rapid and effective means to impact large populations.

NARAC responds to toxic industrial chemical spills, nuclear-power plant accidents, fires, chemical/biological agents, radiological dispersal devices (RDDs), nuclear detonations, and some natural airborne hazards.

NARAC Responds to a Wide Range of Real-World Events



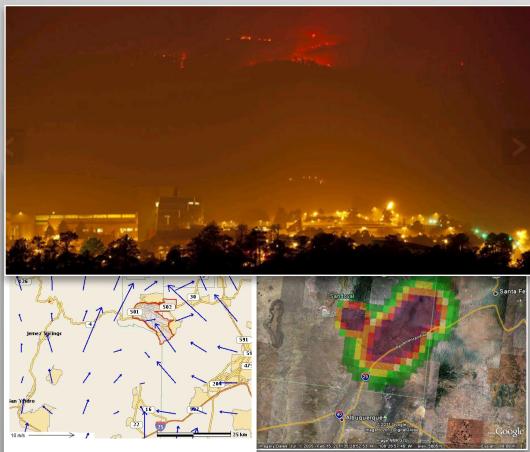
April 26, 1986
Chernobyl nuclear power plant accident



May-June, 2010 in-situ burns
Deepwater Horizon, Gulf of Mexico



March 11 – May 28, 2011
Fukushima Dai-ichi Nuclear Power Plant accident



June 26 - July 1, 2011
Las Conchas Wildfire, NM



November 26, 2011
Mars Science Laboratory Launch, Cape Kennedy, FL



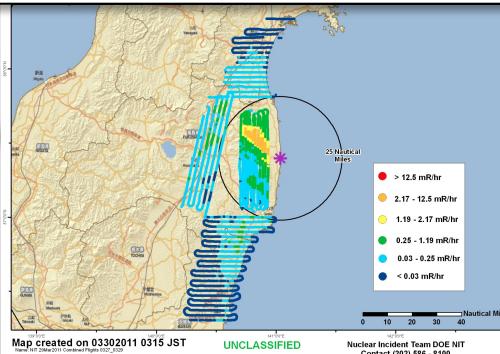
February 14-20, 2014
Waste Isolation Pilot Plant radioactivity venting

Source Estimation and Model Refinement Based on Field Data Is Conducted Iteratively Until Impacts are Characterized

Initial Model Predictions
Guide Measurement
Surveys



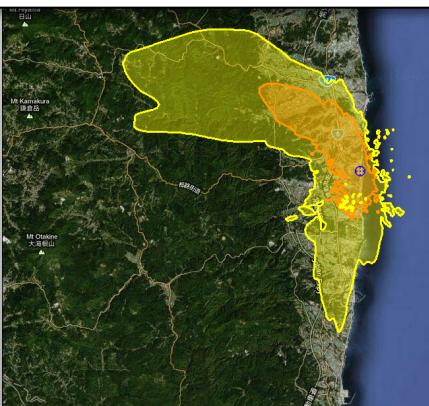
Measurement surveys and sensor data, e.g., DOE AMS, DOE, DoD, local agency field data



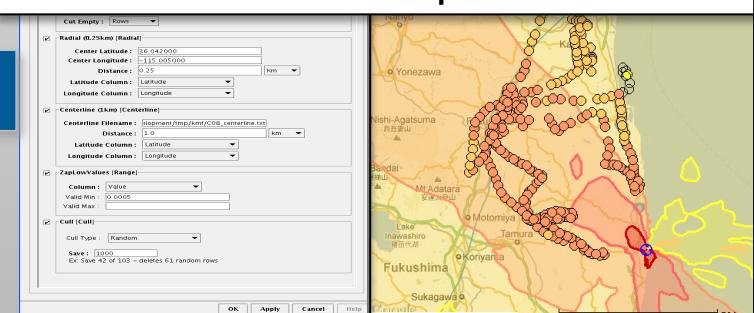
Measurement Data transferred electronically to LLNL/NARAC

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<lon>141.019433
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```

Updated predictions using measurement data



Software used to help select, filter and statistically compare measurements and predictions



Component-based NARAC Computer Systems at LLNL

Support In-house and External Users

LLNL Computer Systems

Central System: Automated model set-up and execution software

Weather Data & Forecasts	Geographic/Terrain Data	CBRN Material Property Data	Dose/Risk Factor Data	Measurement Data
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Source models

3-D Meteorological, Dispersion and Fallout Models

Prompt Effects Models

Data-driven modeling tools

Mapping and product generation software

Population, casualty and fatality estimation

Remote Access Computer System



User interfaces and Analysis Tools for LLNL scientists



Internet/Intranet



Standalone models and mapping



External User Tools
CM/NARAC/IXP Web

- Over 400 software applications
- 50 databases
- 3 million lines of computer code
- 28 servers
- 8 data storage systems

Suite of NARAC Models Are Used to Predict the Consequences of Hazardous Releases (Operational Rad/Nuc Example)

Nuclear Detonation source models:

- LLNL KDFOC
- LLNL LWAC
- ORNL ORIGEN
- ORNL DELFIC



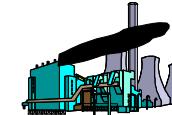
RDD Source models:

- SNL Source Term Calculator
- SNL PUFF
- SNL ScatterMe



Nuclear power and fuel sources:

- NRC RASCAL



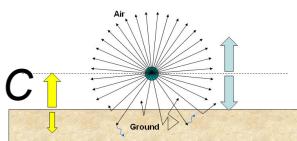
Fire source model:

- LLNL

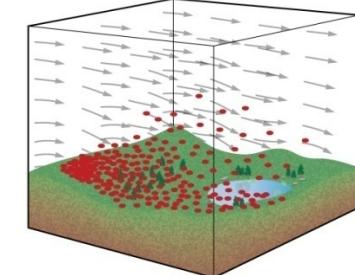


NucDet (IND) and RDD Prompt effects models:

- SNL Nuke
- SNL Blast
- LLNL LWAC

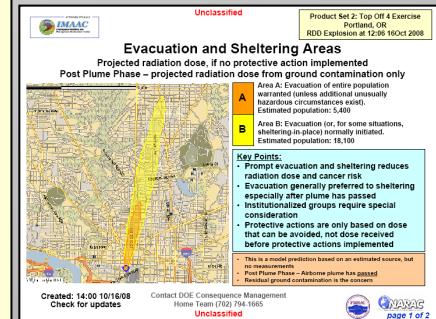
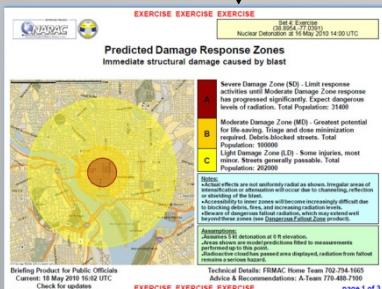


3-D Atmospheric Dispersion and Fallout models: LLNL ADAPT/LODI



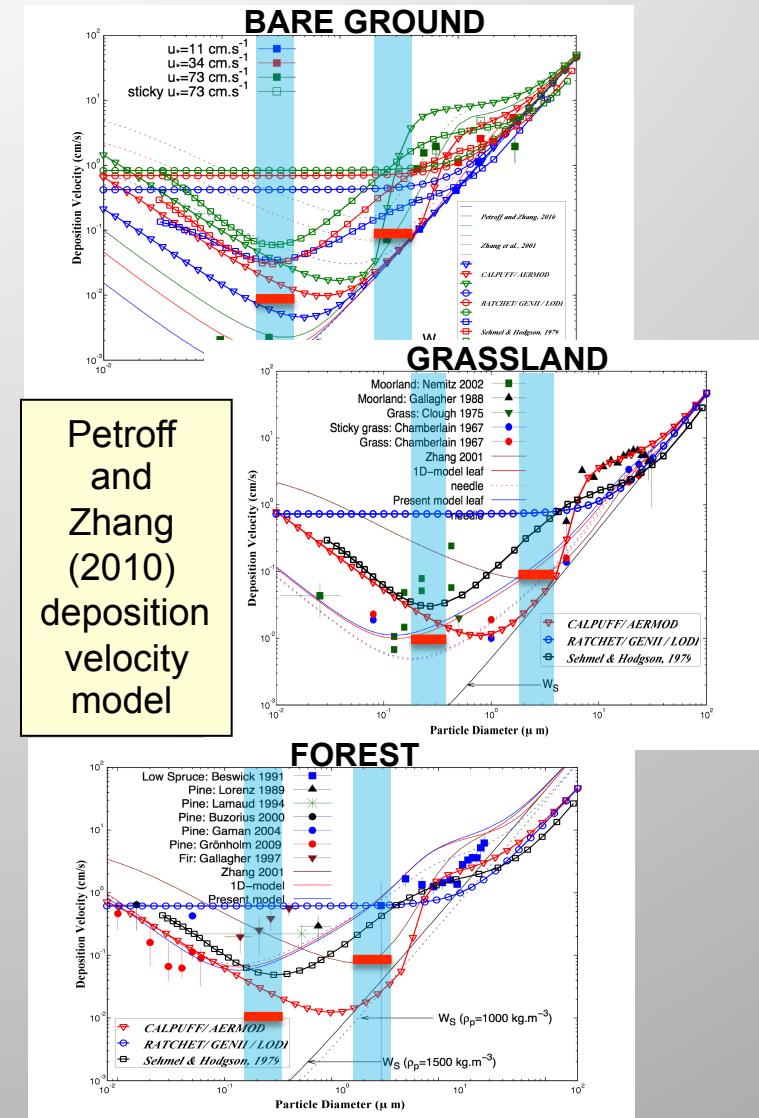
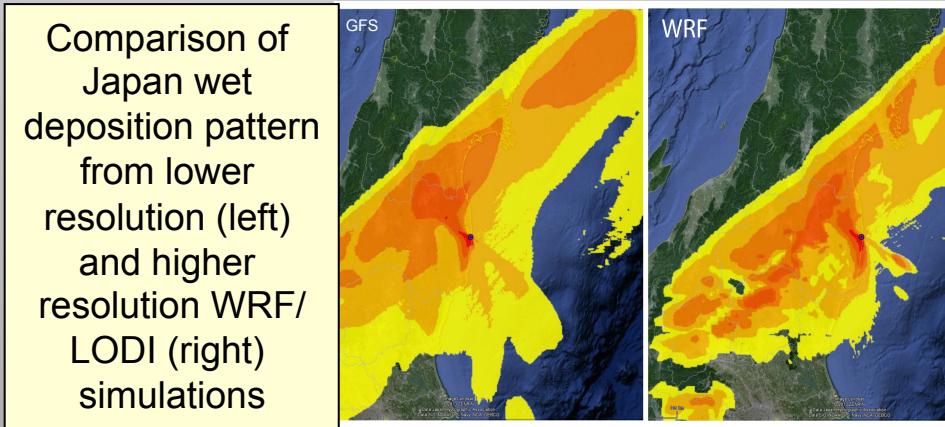
Products:

- Airborne and ground contamination for public exposures (evacuation / sheltering, relocation)
- Affected population and casualty estimates
- Worker protection (stay times)
- Building damage from blast overpressure
- Radiation, blast and thermal casualty estimates
- Neutron-activation ground shine dose



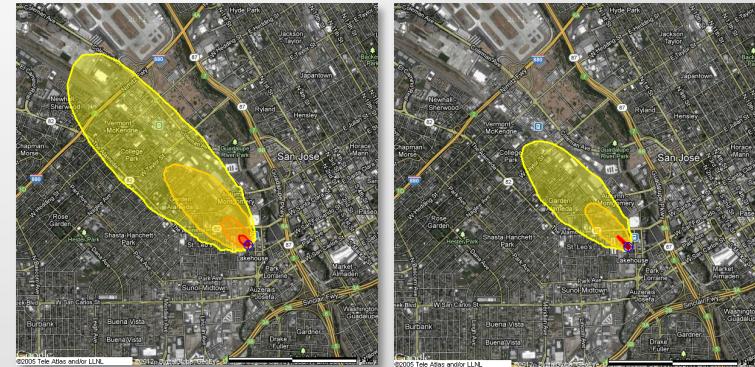
Development Priority: Improved Meteorological and Dispersion Model Physics and Fidelity

- Numerical weather prediction (NWP) modeling enhancements (key to accurate modeling of Fukushima Dai-ichi nuclear power plant accident)
 - Higher-resolution NWP simulations
 - Meteorological data assimilation (4DDA)
 - Use of extended set of NWP precipitation data
- Dispersion processes: deposition
 - In-cloud and below-cloud precipitation scavenging
 - Petroff and Zhang (2010) dry deposition velocity for particles
 - Gaseous dry deposition mode
 - Maxwell and Anspaugh resuspension model (2011)

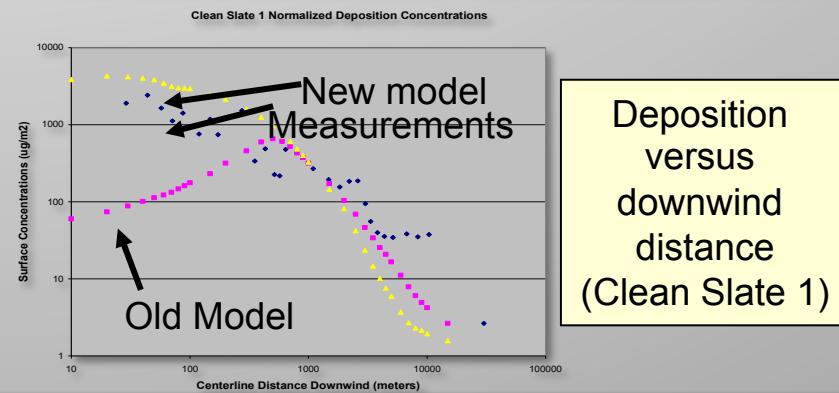


Model Development Priorities: Radiological Dispersal Device (RDD) Model Enhancements Based on Experimental Studies

- Ballistic particles (>100 mm) ejection from the thermally buoyant cloud (SNL experimental studies)
- Explosive particle size distribution for different surfaces
- Dynamic cloud rise
- Particle-cloud coupling
- Experimental results from on-going Israeli Green Field (GF) and Canadian RDD field experiments
 - Improved cloud-top heights for lower high explosive amounts
 - Validation of (RDD) modeling
- Areas for future investigation
 - Particle / activity size distributions for different environments
 - Effects of urban environments on RDD cloud rise

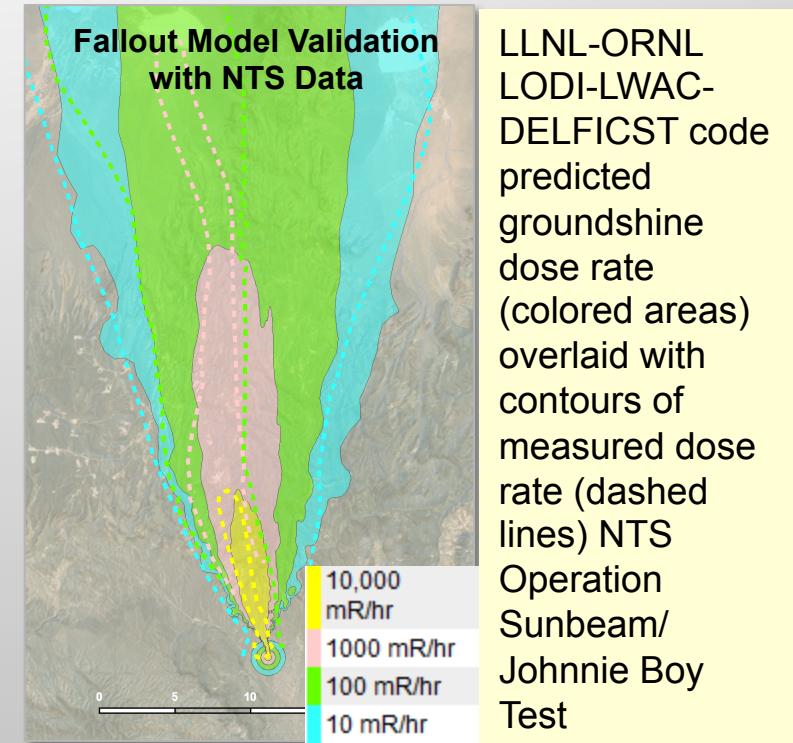


LODI predicted ground-shine dose without (left) and with (right) ballistic particle correction for a source uses 30% 0.1-100 μm and 70% 100-1000 μm particles. Ballistic particle correction increases near-source concentrations but reduces downwind contamination levels.



Development Priority: Higher Fidelity Nuclear Detonation Modeling for Response and Forensics Applications

- Nuclear detonation source terms
 - Radionuclide inventories (ORNL/ORIGEN fission products) and neutron activation products (LLNL/LWAC)
 - Dynamic cloud rise (ORNL/DELFICST and SNL/ERAD)
 - Particle/activity-height distributions and cloud geometry (LLNL/KDFOC, ORNL/DELFICST)
 - Fallout fractionation (different particle/activity size distributions for volatile and non-volatile)
- New products for nuclear forensics applications (sample collection guidance)
 - Total fallout debris mass
 - Equivalent fissions
 - Specific abundance
 - Fractionation ratios
 - Nuclide or mass chain total deposition
- Future model development
 - Non-desert environments (urban, water)
 - First principles cloud rise, particle formation, and cloud-coupling methods

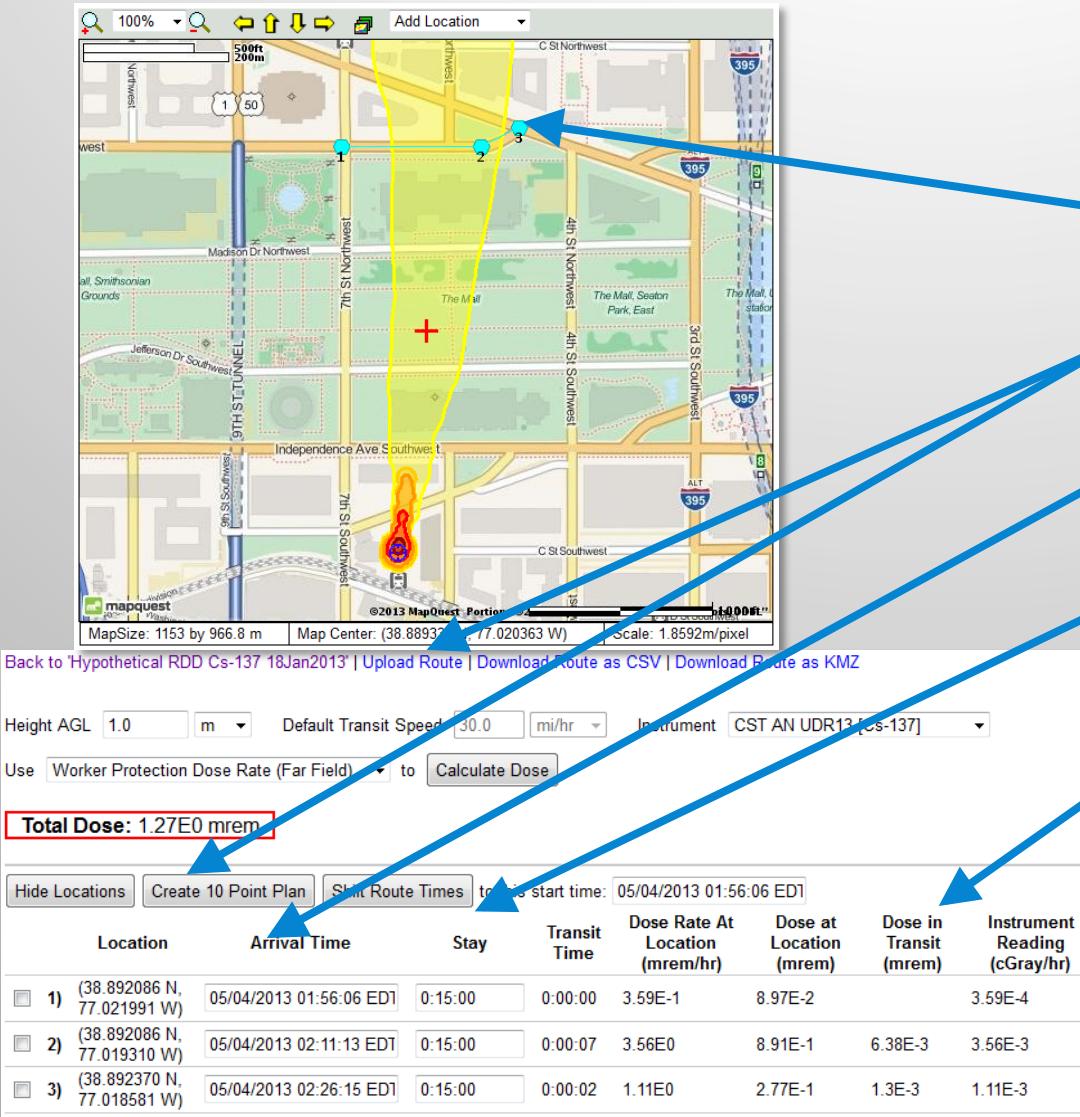


Development Priority: Advanced Nuclear Power Plant Scenarios and Source Term Exchange Formats

- Collaborative effort with US Nuclear Regulatory Commission (NRC) for nuclear power plant accidents
 - Expanded electronic files to share/import complex nuclear power plant release information into NARAC model simulations
 - Default set of nuclear reactor release scenarios
 - Exploratory efforts to determine whether/how SNL's MELCOR severe accident analysis code could be effectively coupled to atmospheric dispersion models

		Ci
Real World		
Chernobyl		2.1E+08
Fukushima		1.2E+07
Three Mile Island		2.5E+06
Tomsk Reprocessing Plant		6.8E+02
Windscale Fire		3.4E+05
RASCAL Workbook		
Assessing a PWR Core Damage Accident		
PWR/BWR Examples		1.9E+05
PWR		1.3E+06
Station Blackout, Containment Leakage	1.6E+05	
Station Blackout, Steam Generator Tube Rupture	7.2E+08	bs/in2
Station Blackout, Containment Bypass	3.0E+08	bs/in2
Loss of Coolant Accident, Containment Bypass	4.0E+07	re 5 lbs/in2
Loss of Coolant Accident, Containment Leakage	1.0E+05	ssure 5 lbs/in2
Loss of Coolant Accident, Steam Generator Tube Rupture	6.1E+08	e 5 lbs/in2
Coolant Release, Steam Generator Tub Rupture	2.4E+02	
Coolant Release, Containment Bypass	5.0E-01	
BWR		
Station Blackout, Containment Bypass, Release from Reactor building	4.9E+08	
Station Blackout, Containment Bypass, Release via Standby Gas Treatment System	3.5E+08	
Station Blackout, Dry Well, Release from Reactor building	5.2E+05	
Station Blackout, Dry Well, Release via Standby Gas Treatment System	3.1E+05	
Station Blackout, Suppression Pool, Release from Reactor building	3.1E+05	
Station Blackout Suppression Pool, Release via Standby Gas Treatment System	3.1E+05	
Coolant Release, Containment Bypass, Release from Reactor building	2.4E+00	
Coolant Release, Containment Bypass, Release via Standby Gas Treatment System	2.0E-02	
Loss of Coolant Accident, Containment Bypass, Release from Reactor building	1.7E+08	
Loss of Coolant Accident, Containment Bypass, Release via Standby Gas Treatment System	6.6E+07	
Loss of Coolant Accident, Dry Well, Release from Reactor building	4.4E+05	
Loss of Coolant Accident, Dry Well, Release via Standby Gas Treatment System	3.6E+05	
Loss of Coolant Accident, Suppression Pool, Release from Reactor building	3.6E+05	
Loss of Coolant Accident, Suppression Pool, Release via Standby Gas Treatment System	3.6E+05	

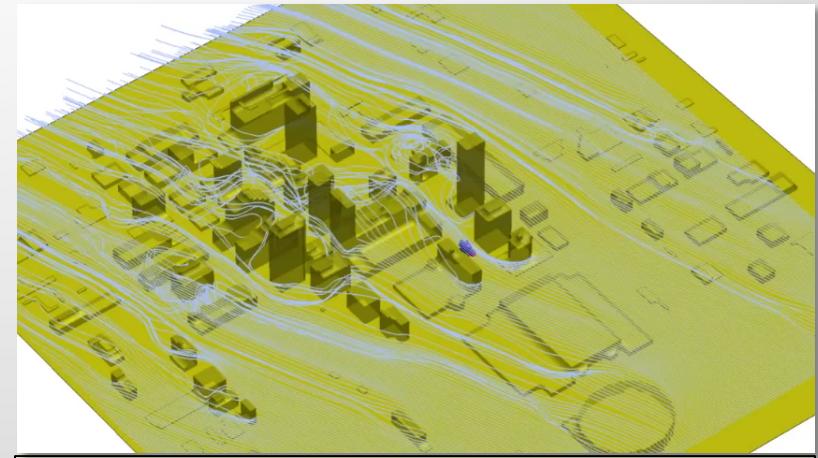
Development Priority: Tools to Support Field Teams (Example Web-based Mission Planning Tool)



- Estimate potential dose bases on route and stay times
- Select route by clicking on monitoring route points
 - Upload monitoring route or use DOE “10 Point Plan”
 - Edit arrival times and stay times
 - Shift route times to account for time variation of groundshine dose
 - Display calculated dose rate, dose, instrument readings
 - Extensions: aerial monitoring and evacuation planning

Development Priorities: Complex Terrain and Urban Models For Operational Applications

- Urban canopy models based on area-averaged parameterizations
- Diagnostic / empirical urban models (e.g., LANL/QUIC)
- First principle's physics models (LLNL/Aeolus)
 - Building-resolving computational fluid dynamics (CFD) coupled to Lagrangian dispersion model
 - RANS and LES solutions
 - Particulate, gas, and denser-than-air gases
 - Rapid automated grid generation from building database (NGA/USGS data)
 - Computational performance suitable for operational applications



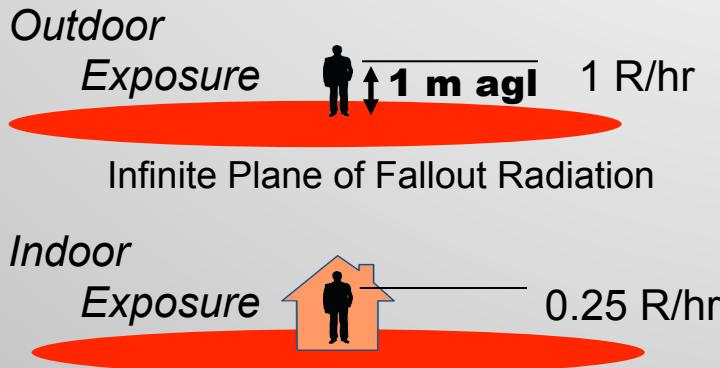
Aeolus fast-running Reynolds Averaged Navier-Stokes (RANS) steady state solution



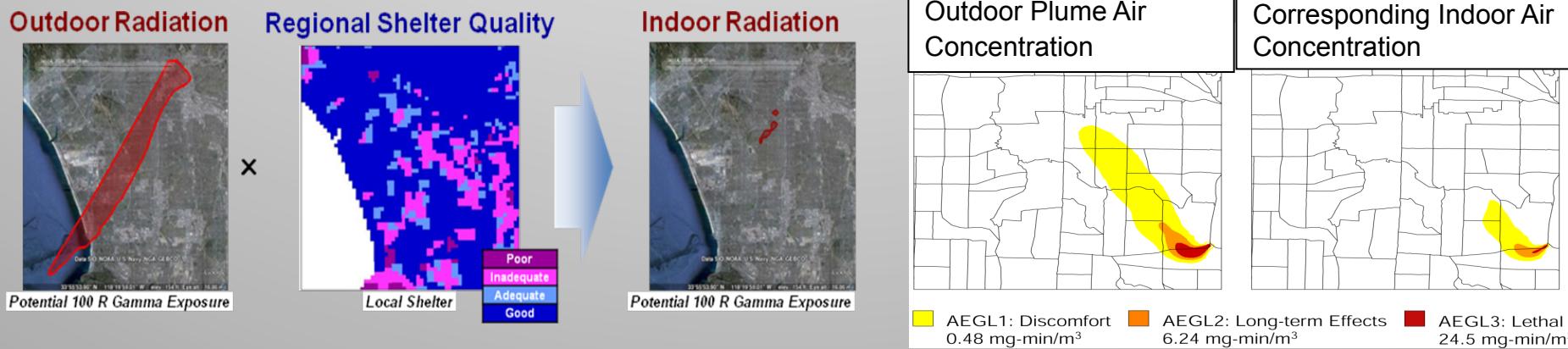
High fidelity time-dependent Aeolus Large Eddy Simulation (LES) including deposition

Development Priorities: Improved Casualty Estimates Based on Sheltering/Shielding and Building Infiltration

Building Protection Factor = ratio of outdoor/indoor exposures = 4



- Modeling of building sheltering/shielding to calculate indoor dose exposures and improve casualty estimates
 - LLNL *PFscreen* model provides estimates of building protection factors
 - LLNL *Regional Sheltering Analysis (RSA)* tool estimates potential protection from gamma radiation for a variety of shelter strategies based on existing database of building properties (e.g., FEMA HAZUS data)
- Building infiltration models and building leakiness databases based on statistical relationships and US Census data (with LBNL)

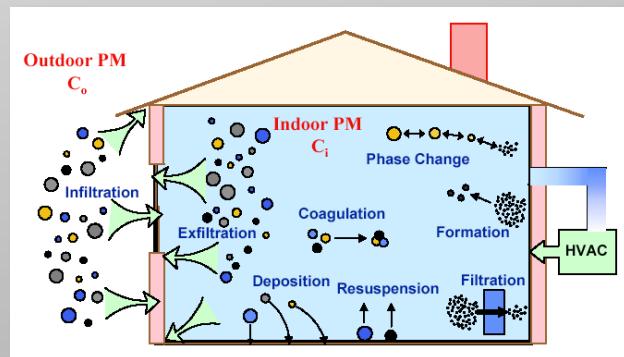


Development Priority: Coupled Subway / Indoor Models with Atmospheric Dispersion Models

- ANL: 1D advection-diffusion equation subway transport and dispersion model
 - Tunnels, large “rooms”, entrances
 - Piston and wake effect of trains
 - Transport by train cars
 - HVAC exhaust fans, leakage
 - Natural flows and mechanical ventilation
 - Validated with experimental studies
- Subway model coupled to urban models (LANL/QUIC; LLNL/Aeolus) models
- LBNL: multi-zone models (e.g., NIST/CONTAM) for whole building transport and CFD models for individual rooms
 - Conditions at building envelope
 - Indoor airflow and HVAC systems
 - Sorption to surfaces
 - Particle filtration, tracking, resuspension, and coagulation



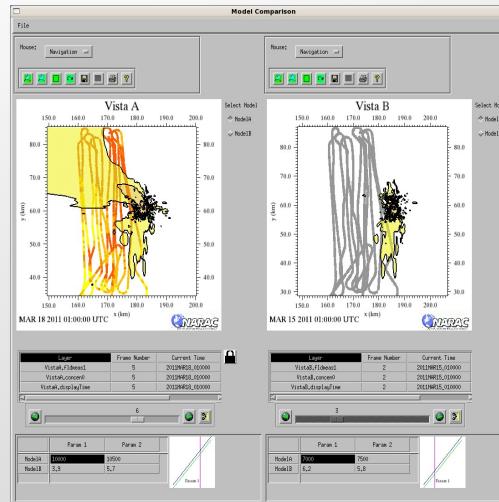
Coupled ANL subway and QUIC outdoor empirical urban model for fictitious system (courtesy of David F. Brown, ANL)



Indoor model processes
(courtesy of Michael Sohn, LBNL)

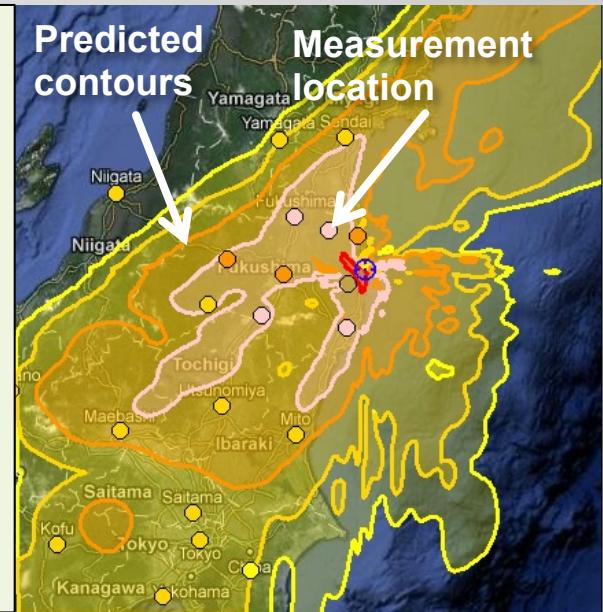
Model Development Priorities: Data Assimilation and Uncertainty Estimation

- Measurement-model integration
 - Numerical weather prediction data assimilation
 - Field-data acquisition including quality assurance
 - Software to rapidly process measurement data
 - Automated sampling of range of potential scenarios consistent with all available information
 - Improved data-model statistical/graphical comparison and analysis tools to support expert source estimation analyses
- Uncertainty estimation
 - Ensembles (meteorological and dispersion)
 - Source estimation methods
 - Quantitative rigorous uncertainty estimation (source term, meteorology, dispersion processes)



- Model-data analysis tools
- Automated sampling of input parameter
 - Data-model paired in space time
 - Statistics: FB, RMSE/NMSE, StdDev, GMV, factor of R, etc.
 - Graphical model-data comparisons

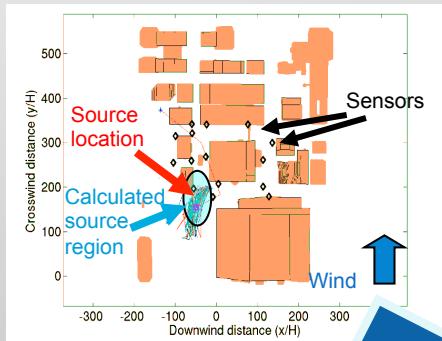
NARAC model predicted dose rate compared to MEXT data for March 15, 1800 UTC. Colors code: $120\mu\text{Gy h}^{-1}$ (red), $4\mu\text{Gy h}^{-1}$ (pink), $0.4\mu\text{Gy h}^{-1}$ (orange), $0.04\mu\text{Gy h}^{-1}$ (light orange) and $0.004\mu\text{Gy h}^{-1}$ (yellow).



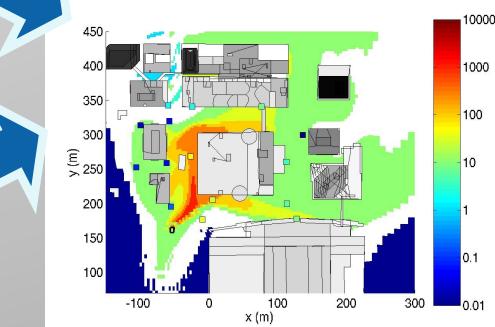
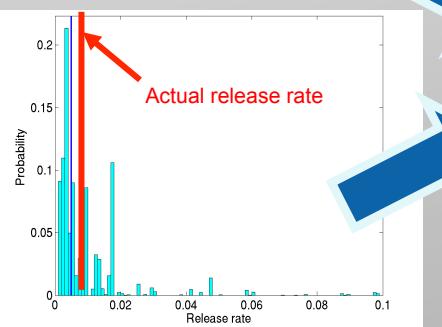
Development Priorities: Robust Statistically-Rigorous Source Estimation Methods Using Field Data

- Backward trajectory methods (accounting for null data)
- Minimization of cost functional
- Source-receptor optimization starting with *a priori* estimate (“predictor-corrector”)
- Adjoint modeling (not used)
- Bayesian inferencing and stochastic sampling
 - Backwards analyses to determine probabilistic distribution of unknown source characteristics
 - Optimal forward predictions for consequence assessment
 - Dynamic reduction in uncertainty as additional data become available
 - Complex sources (e.g., multiple, moving)

NARAC chemical odor source location analysis based on backward trajectories

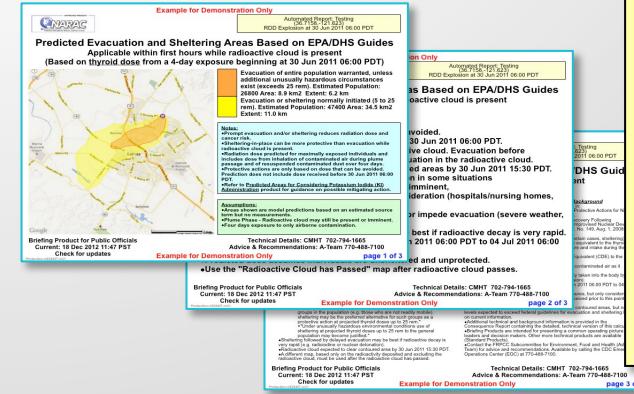


Bayesian inference and stochastic sampling estimates release rate and source location for the JU2003 Oklahoma City release and generates the 90% confidence level composite plume below (field data shown by colored squares).



Development Priorities: Products for Communication with Users Developed with Interagency Input

- Standard suites of CBRN technical products showing plume hazard areas, affected populations, health effects, protective action guide levels, and geographical information
- Consequence reports documenting results, inputs, assumptions, and plot interpretation
- Interagency-developed Briefing Products for decision makers and emergency responders focused on actions that need to be considered to protect the public and the environment
 - Evacuation / shelter-in-place, relocation, worker protection, agricultural embargo
 - Operational products: radiological dispersal devices, nuclear detonations, nuclear power plant accidents
 - Draft versions: toxic industrial chemicals, chemical/biological agents
- Supplementary analyses (meteorology, deposition, field data, animations)
- Product output in multiple formats for integration into user's GIS systems

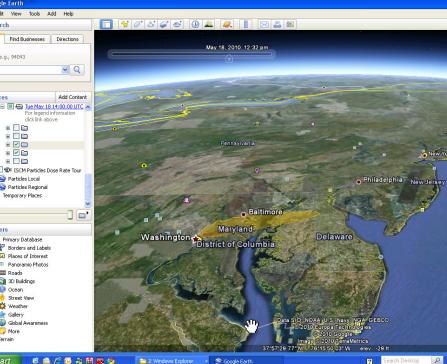


Briefing products for radiological dispersal devices, nuclear detonations, nuclear power plant accidents, CB releases



Animations and time series plots to display evolving impacts

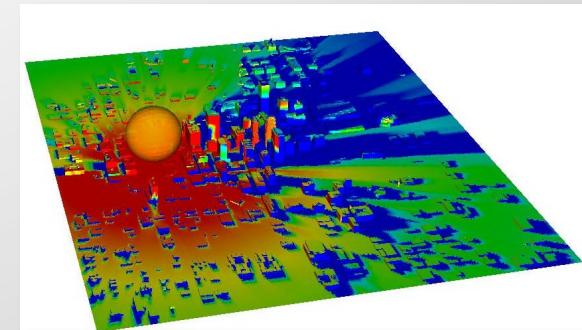
PDF, PowerPoint, HTML/XML, JPG/PNG graphics
ESRI Shape and Google Earth KMZ GIS files with plume areas



Briefing Products: Kevin Foster, Kristen Yu (LLNL),
Harvey Clark (RSL)

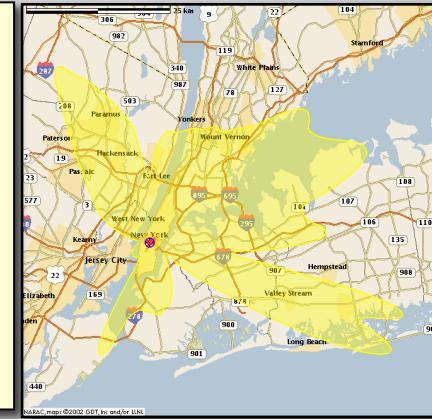
On-Going Atmospheric Dispersion Modeling Challenges

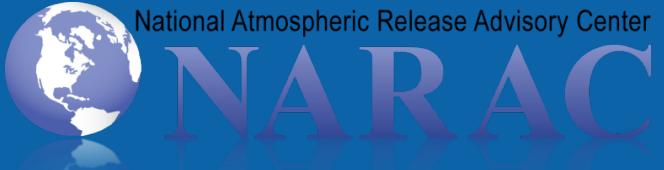
- Meteorological and dispersion model improvements
 - New validated CBRNE source models
 - Meteorological process: precipitation, turbulence, vertical mixing, land-sea breezes
 - Physical processes: deposition, phase/chemical changes, resuspension
 - Effects of urban and other environments
- Data assimilation
 - Numerical weather prediction data assimilation
 - Use of non-traditional (e.g. remote sensing) data and/or information sources
 - Rigorous quantitative tools and methods for source/event reconstruction and data fusion
 - Uncertainty estimation
- Data for real-world response and model testing
 - Standardized field data (collection methods, data exchange formats, metadata, quality assurance)
 - Open-access field experiment databases with quality-assured data and documentation
- Communicating technical information and uncertainties to planners, decision makers, and emergency responders



Prompt thermal energy from a nuclear explosion in an urban environments (courtesy of Ross Marrs, LLNL)

Example showing variability of fallout dose pattern for New York City from multiple weather conditions (Kevin Foster)





Web: narac.llnl.gov
Email: narac@llnl.gov

Contributors to material in this briefing: John Nasstrom, Brenda Pobanz,
Shawn Larsen, Michael Dillon, Kevin Foster, Peter Goldstein, Akshay
Gowardhan, and Matthew Simpson

Backup / Supplemental Slides

NARAC Provides Operational Services, Tools, and Expertise for Preparedness, Response, & Recovery

Event Information

- Weather data
- Nuclear, radiological, chemical, and biological source information
- Terrain, land use, and population databases
- Measurement data and observations



Operational Services and Expertise

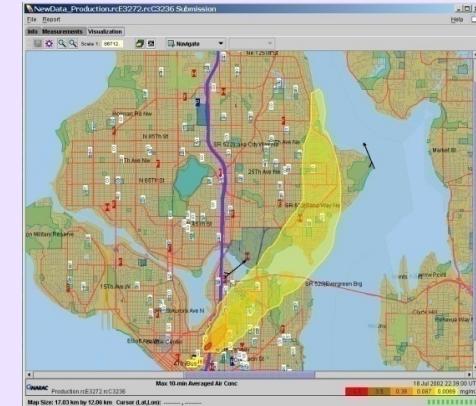
- Suite of stand-alone to advanced WMD modeling tools (multi-scale models)
- 24/7/365 expert scientific staff (< 5 min. reach-back)
- Detailed analysis, expert interpretation, quality assurance, and training
- Event reconstruction



Photo Courtesy of Tracy Press

Actionable Information

- Hazard areas and affected populations
- Health effect, public protective action, and worker protection levels based on federal guidelines
- Casualty, fatality, and damage estimates
- Planning and consequence assessments



Center Responds to Real-World Emergencies



May 25-26, 2004
chemical warehouse fire
in Conyers, GA



July 28, 2005 solvent
plant industrial fire in
Ft. Worth, TX



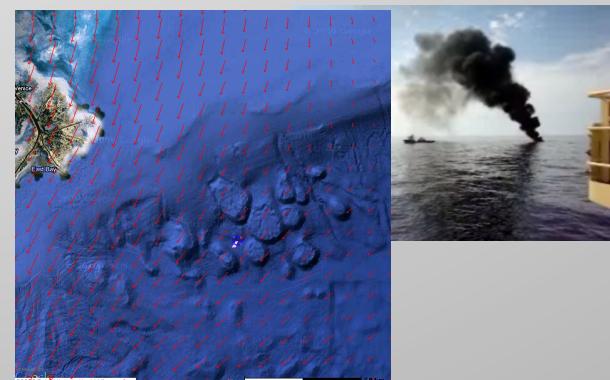
July 17, 2007
Barton solvents fire
in Valley Center, KS



Jan 16, 2007 train
derailment fire in
Shepherdsville, KY



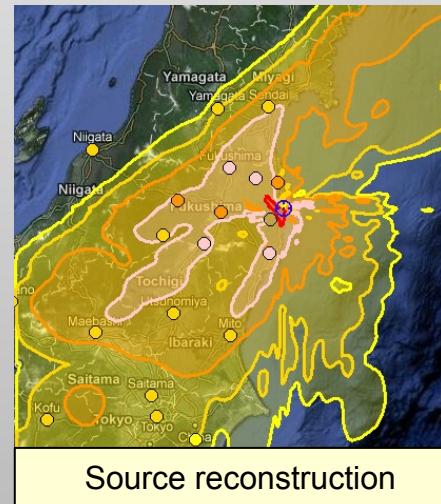
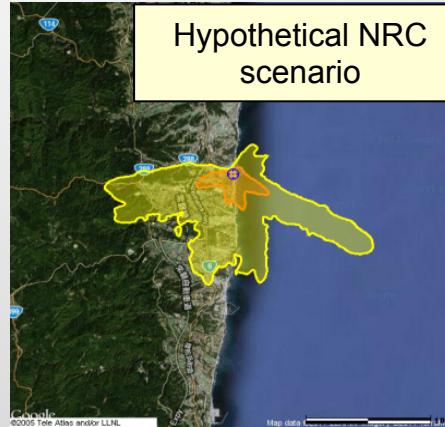
April 7-10, 2008 Kilauea,
Hawaii sulfur dioxide
releases



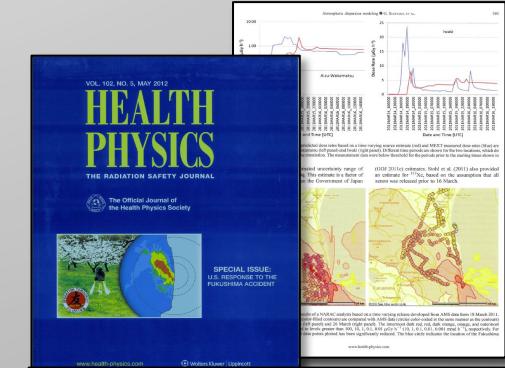
May-June, 2010 Deepwater
Horizon in-situ burns,
Gulf of Mexico

NARAC Supported A Variety of Requests During the Fukushima Response (March 11-May 28, 2012)

- Daily weather forecasts to support mission planning and situational awareness
- Estimates of possible dose in Japan based on hypothetical U.S. Nuclear Regulatory Commission radionuclide release scenarios to support protective action planning for U.S. citizens in Japan
- Predictions of possible arrival times and dose levels at U.S. locations
- Source term estimation and plume model refinement based on field data

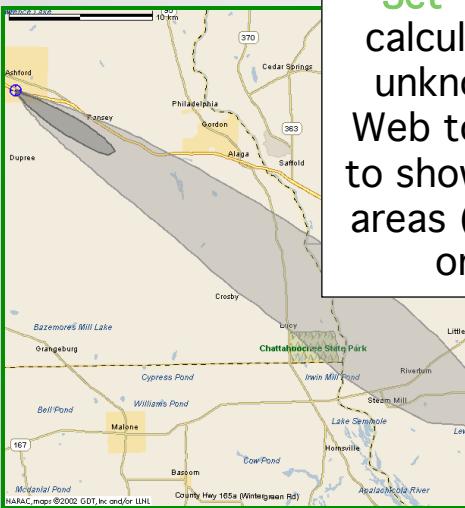


Arrival time and potential dose levels in U.S.

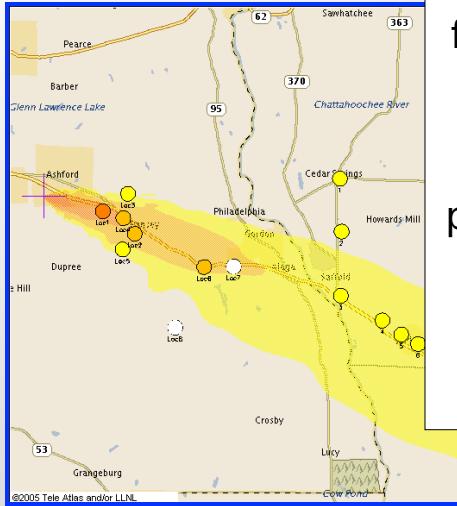


Sugiyama et al., 2012: *Health Physics*, 102, p 493–508

Standard Operational Procedures Couple Modeling and Monitoring in a Cyclical Process



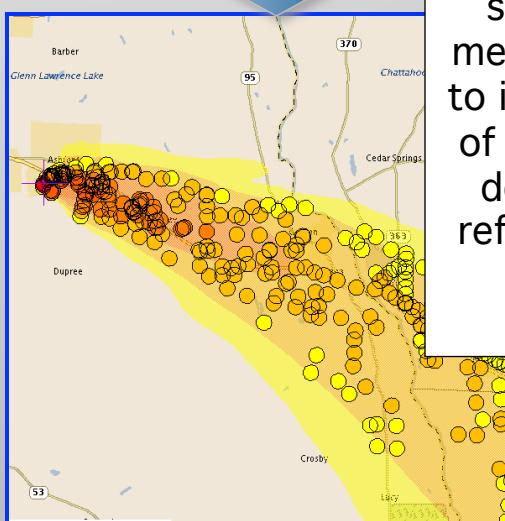
Set 1. Initial automated calculation can be run for unknown material (using Web tools or NARAC staff) to show downwind affected areas (no estimate of dose or health effects)



Set 2. Initially available field measurements are used to refine NARAC model inputs (e.g., source amount) and predictions to produce a preliminary estimate of dose for evacuation / sheltering protective action guides



Later Sets:
Model predictions combined with measurement surveys are used to develop longer range relocation protective action guide and food-ingestion dose plots

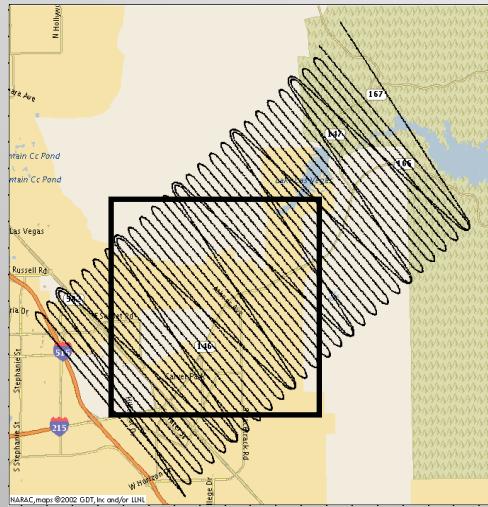


Set 3+. More extensive sets of FRMAC/AMS measurements are used to improve the accuracy of the source term and dose predictions for refining evacuation and sheltering guides (*iterative process*)

Automated Field Measurement Processing Reduces Delivery Time for NARAC Data-Model Products

Monitoring / Field Data

- Multi-agency data / databases
 - Electronic data acquisition
(standardized and custom formats)



Aerial Measurement - Gamma Spectroscopy

In situ field assays – Gamma Spec,
Alpha/Beta Survey, Dose Rate
Air Filters (paper, charcoal) – Gamma
Spec, Alpha/Beta Counters, Lab
Analysis
Soil and Soil Cores – Gamma Spec,
Lab Chemistry

The screenshot displays the DataFilter, DataStats/DataScaling software interface. On the left, a 'Development: Filters' panel shows several filter configurations:

- EmptyRows (Cut):** Cut Empty: Rows
- Radial (0.25km [Radial]):** Center Latitude: 56.042000, Center Longitude: -115.005000, Distance: 0.25 km, Latitude Column: Latitude, Longitude Column: Longitude.
- Centerline (1km [Centerline]):** Centerline Filepath: /tmp/kml/CO8_centerline.kml, Distance: 1.0 km, Latitude Column: Latitude, Longitude Column: Longitude.
- ZapLowValues (Range):** Column: Value, Valid Min: 0.0005, Valid Max: .
- Cull (Cull):** Cull Type: Random, Save: 1000, Ex: Save 42.

Below the filters is a 'Model Comparison' section with two side-by-side plots:

- Vista A:** A map showing a complex trajectory over a geographic area from March 18, 2011, at 01:00 UTC. The plot includes a yellow shaded region and a black trajectory line.
- Vista B:** A map showing a similar trajectory over the same period and area, with a yellow shaded region and a black trajectory line.

At the bottom, there are two tables for model comparison:

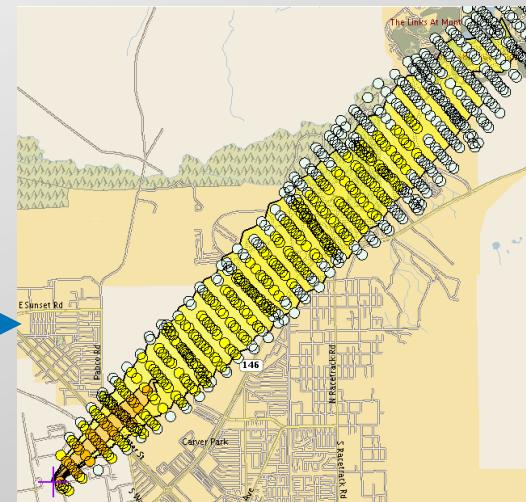
Layer	Frame Number	Current Time
VistaA/fileseq	5	2011MAR05_000000
VistaA/concen	5	2011MAR05_000000
VistaA/displayTee	5	2011MAR05_000000

Layer	Frame Number	Current Time
VistaB/fileseq	2	2011MAR05_000000
VistaB/concen	2	2011MAR05_000000
VistaB/displayTee	2	2011MAR05_000000

DataFilter, DataStats/ DataScaling

- Filtering, grouping, outlier elimination
 - Background corrections
 - Source ratio scaling

Data-Model Comparisons Refined Model Predictions

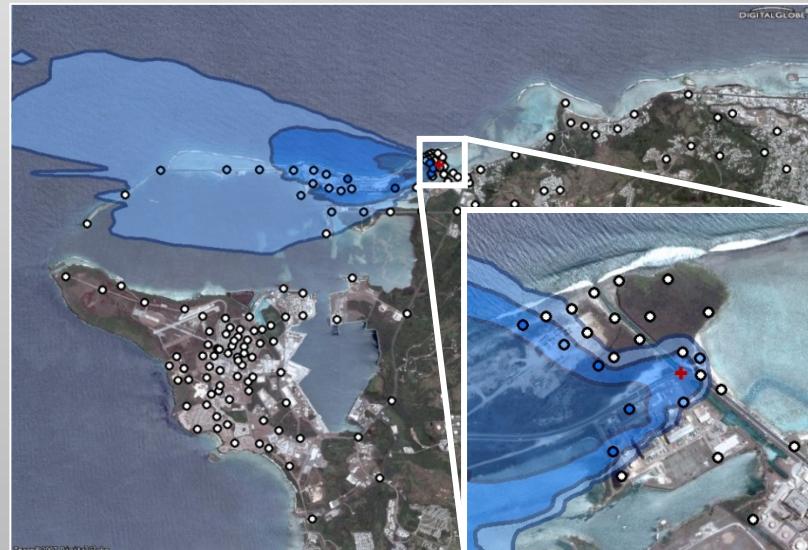
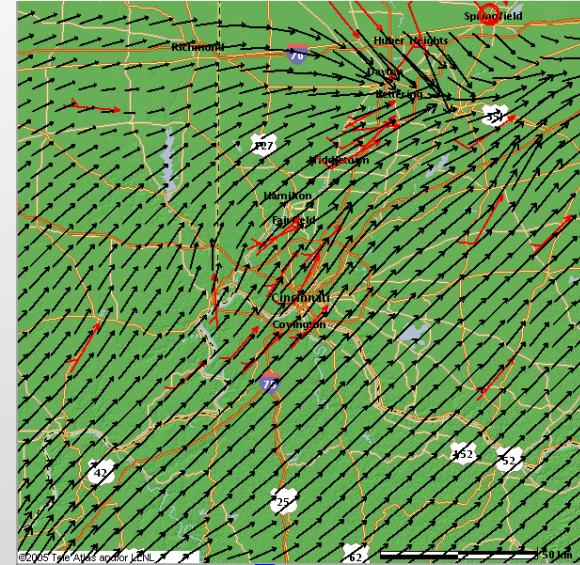


Graphical/Statistical Data/ Model Comparison Tools

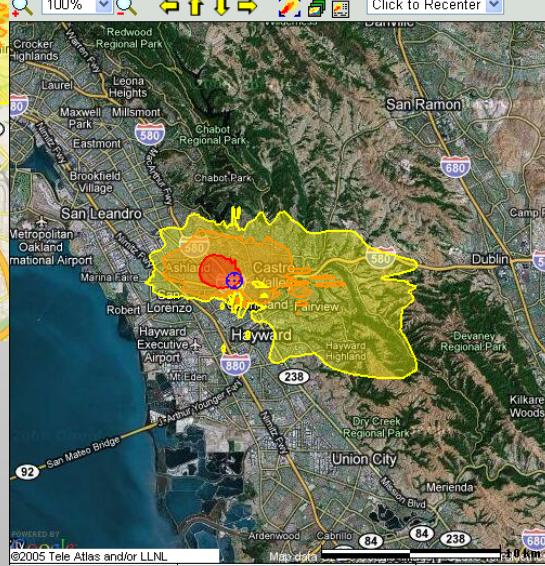
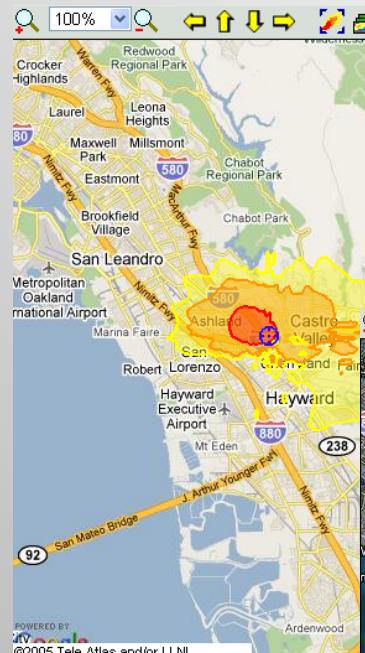
- FB, MG, NMSE, VG, Factor of R
 - Measurement map displays
 - Graphical model-data
 - Data-model comparisons (paired in space time)

Auxiliary Analyses Are Provided For Situational Awareness

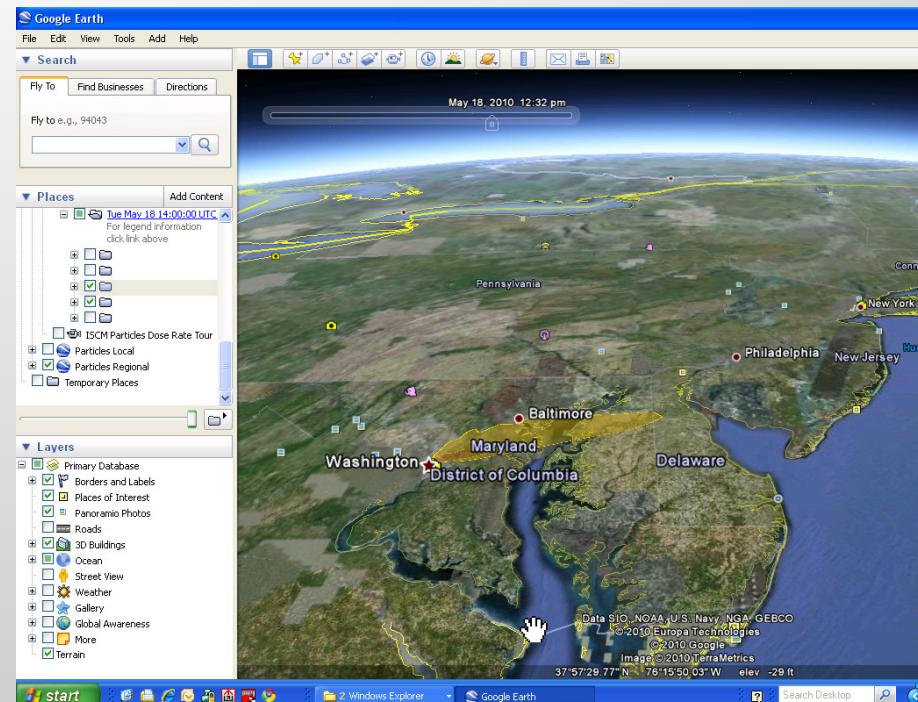
- Wind observations and fields
- Numerical weather prediction forecasts
- Field measurement data
- Deposition
- Time series, particle, or plume animations



Products and Map Layers are Provided in Multiple Formats (PDF, ESRI, Google)



Worldwide Google Street and satellite displays



Export plumes to Google Earth (FEMA)

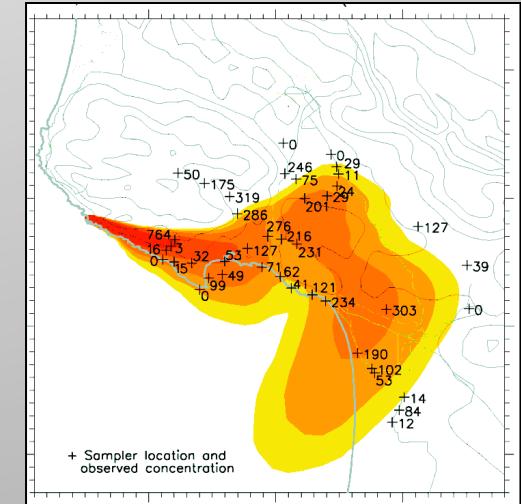
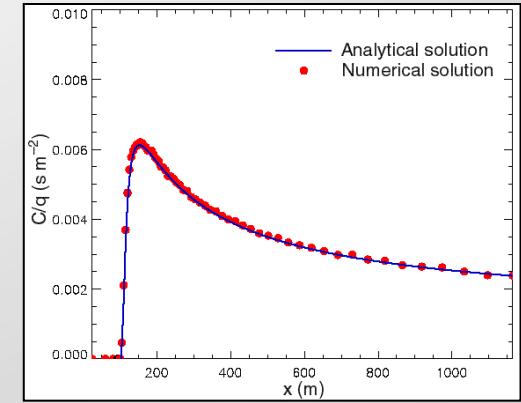
Available on NARAC/CM Web
PDF, PowerPoint, HTML/XML, JPG/PNG graphics,
ESRI Shape and Google Earth KMZ GIS files with
plume areas

Model Development Drivers (NARAC Perspective)

- Mission areas requirements (e.g., emergency response, hazard assessment, consequence analysis, FRMAC and other interagency needs, nuclear forensics)
- Customer / user feedback
- Lessons learned from exercises (consequence management, emergency response)
- Experiences in real-world emergencies (e.g., Fukushima)
- NARAC staff expert (tools to support analyses)
- Externally driven updates to databases and data feeds (geographical, hazardous material, meteorological, CBRN field data, health effects / dose response)
- S&T development (internal model development, integration of externally-developed capabilities, external collaborations)
- Interagency collaborations and partnerships

Model Validation is an On-Going Process Involving Multiple Components and Real-World Events

- Multiple validation components
 - Analytic comparisons against known results
 - Laboratory experiments validate model physics against experimental data
 - Field studies test models in real-world conditions (statistical and graphical metrics)
 - Operational testing evaluates the usability, efficiency, consistency and robustness of models for operational conditions
- Transferability to operations
 - DOE / LLNL software quality assurance (SQA) standards
 - Extensive testing by in-house analysts and external beta users
- Accreditation
 - NARAC: DOE SCAPA Consequence Assessment Modeling Toolbox for DOE sites (certifies compliance with SCAPA SQA guidance for non-safety applications)
 - HotSpot and EPIcode: DOE Safety Software Central Registry toolbox code (meets DOE Office of Health, Safety, and Security (HSS) Safety SQA criteria)



Data is Needed for Both Real-World Response and Testing of Models

- Environmental monitoring measurement data needs
 - Real-time standardized data collection methods
 - Standard formats and metadata for data exchange
 - Rapid quality assurance
- Additional experimental data needed for model development, testing and validation
 - Dispersion/deposition data for complex meteorology/terrain
 - Urban dispersion
 - Particulate releases
 - Buoyant sources
 - Nuclear fallout data (for conditions different from nuclear test sites)
 - Health effects and dose exposure models, including impacts of compounding injuries
 - Deposition, weathering, degradation, viability, and resuspension data and models
- Long-term open-access field experiment databases with quality-assured data and documentation