Transport and Dispersion Model Options

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The air pollutant health or other effect drives the transport and dispersion (T&D) model approach

- Determined by source scenario and health or environmental or economic or social effect
- Different averaging times
  - SO_2 from power plant stack – EPA regulations start with one-hour concentration at a given point.
  - Radiological gas release from nuclear plant – an issue can be the integrated dose over time and across population.
  - Chlorine from railcar rupture – seconds (one breath) to minutes for lethal or severe health effects.

Current Major Air Pollution Issues

- CO_2 and other global pollutants and climate change
- Long-range transport of pollution from major point source incidents (e.g., large fires, volcanoes, nuclear plant accidents)
- Regional chemically-reactive pollutants (ozone, PM, mercury)
- Short-to moderate distance (< 20 km) industrial plumes
- Mobile sources (traffic, train, ship, airplane, construction)
- Short distance (< 2 km) accidents (chemical processing plant accident, train derailment, chem/bio agents from an urban terrorist attack)

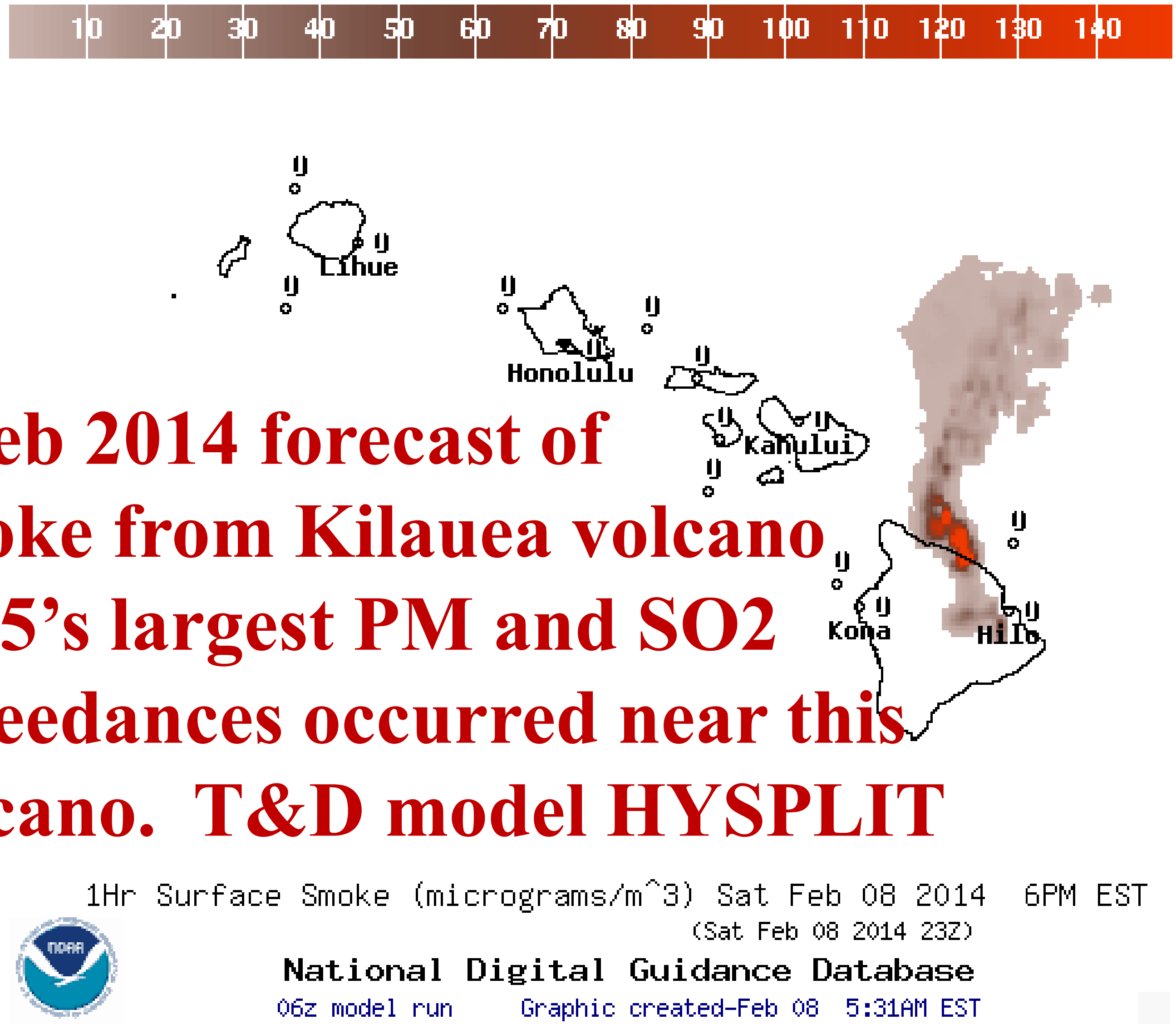
Long-range transport of pollutants from major incidents (e.g., volcanoes, forest fires, nuclear plant accident)

- Many uncertainties; e.g., source emission rate and plume rise
- Most countries have linked meteorological models and transport and dispersion models for this
- In most cases the weather scenario itself leads to uncertainties (e.g., the radiation dose from the Fukushima plume occurred mostly on one day with on-shore winds and showers)
- "Inverse modeling" and Bayesian updating are sometimes used to estimate source magnitude and location based on sampling data.

Iceland's Eyjafjallajokull volcano April 16, 2010

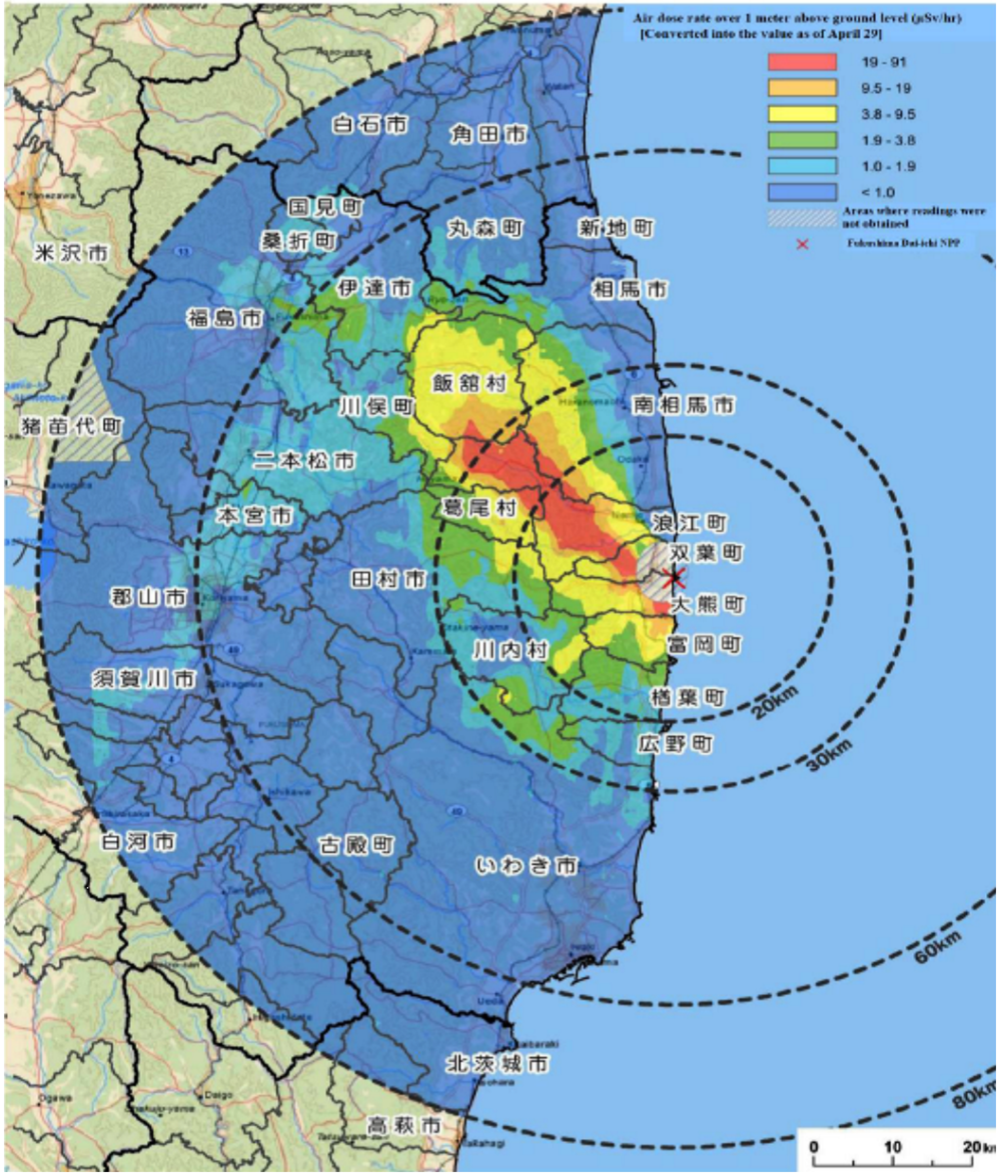
airquality.weather.gov

NOAA web product – surface smoke (micro-g/m^3)



8 Feb 2014 forecast of smoke from Kilauea volcano 2015's largest PM and SO2 exceedances occurred near this volcano. T&D model HYSPLIT

Results of airborne monitoring by MEXT and DOE
(Readings of air dose monitoring inside 80km zone of Fukushima Dai-ichi NPP)



Airborne monitoring shows the pattern of deposition from Fukushima

The major impact occurred during rain showers on 15 March during winds from SE

Transport and Dispersion in the Atmosphere

(Common characteristics that must be accounted for by all T&D models)

- Gases and aerosols comprising air pollution are transported by the mean wind and are dispersed by the ambient turbulence.
- Thus all T&D models require inputs (or parameterizations) of mean winds and turbulence.
- There are thermodynamic effects that require knowledge of plume characteristics and atmospheric stability.
- There may be chemical reactions and/or deposition
- Detailed terrain data and land use are also needed

Categories of T&D Models

- Box or Slab (e.g., $C = (\text{Mass flux})/(u \cdot \text{area})$)
- Simple Gaussian plume or puff (Gaussian or normal distributions away from cloud center)
- Lagrangian particle or puff (particle or puff center moves with wind; dispersion due to turbulent velocities)
- 3-D Eulerian meso- or regional- or global- scale (Solves 3-D time dependent equations of motion and state etc. using finite difference methods)
- CFD (actually a subcategory of 3-D Eulerian, but uses a much smaller 3-D grid volume)

Categories of T&D Models (p 2)

- All categories require weather inputs. Options are
  - Single site
  - Diagnostic mass consistent wind model
  - NWP (3-D weather forecast model such as WRF)
- Examples of T&D models
  - Gaussian plume or puff (AERMOD, MACCS/ATMOS)
  - Lagrangian particle (QUIC, MSS, LODI)
  - Lagrangian puff (SCIPUFF, CALPUFF, RATCHET)
  - Eulerian meso and regional (CMAQ, CAMx)
  - CFD (NCAR, AEOLUS, FLACS, various FLUENT versions)
  - Hybrid – HYSPLIT (Lagrangian puff and Eulerian)

Categories of T&D Models (p 3)

- All T&D models are moving towards the capability to use NWP (e.g., WRF) weather inputs. Some use real-time WRF (such as CMAQ, HYSPLIT, SCIPUFF). This capability is used by most countries.
- Still, most retain the ability to use mesoscale wind networks to develop mass-consistent diagnosed wind fields (e.g., CALMET, SWIFT)
- Uncertainties in model predictions are assessed in two major ways: Monte Carlo methods such as in MAACS, and ensemble methods such as in the European Union ENSEMBLE system developed after Chernobyl and ETEX and hoped for in IMAAC. SCIPUFF directly outputs uncertainties since it predicts the variance in addition to the mean.

IMAAC
Interagency Modeling and Hazard Assessment Center

- Located at LLNL NARAC in Livermore CA until about 2008
- Now at DTRA reachback (Ft Belvoir, VA), which is manned by at least three persons 24/7
- IMAAC coordinates and disseminates Federal atmospheric T&D modeling and hazard prediction products. These products provide the Federal position during actual or potential incidents involving hazardous material releases.

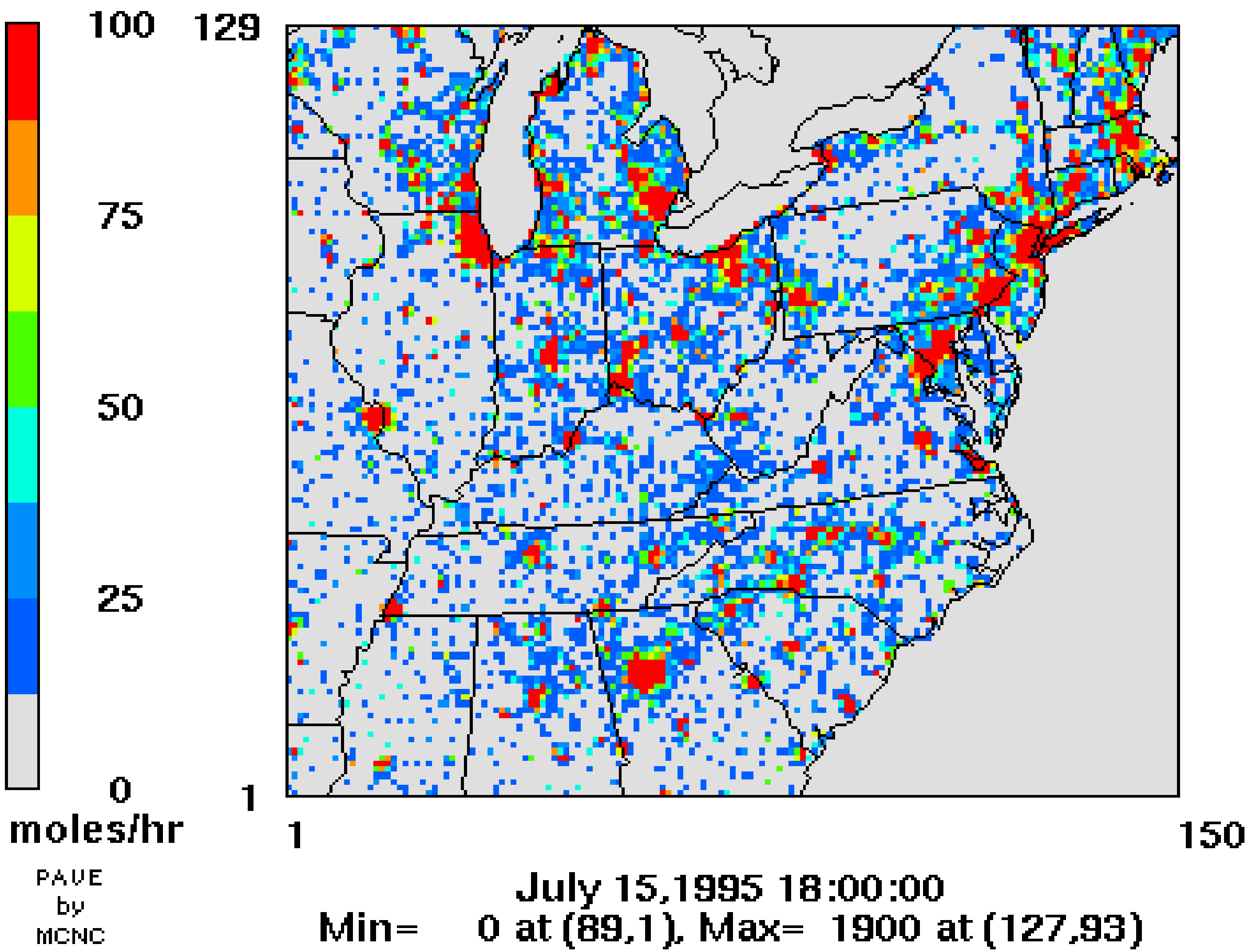
IMAAC continued

- Through plume modeling analysis, IMAAC provides emergency responders with predictions of hazards associated with atmospheric releases to aid in the decision making process to protect the public and the environment
- Must be asked
- Supposedly makes use of T&D models from several agencies. However, usually HPAC/SCIPUFF is used (DTRA's model)
- Possible future use of multi-model ensembles

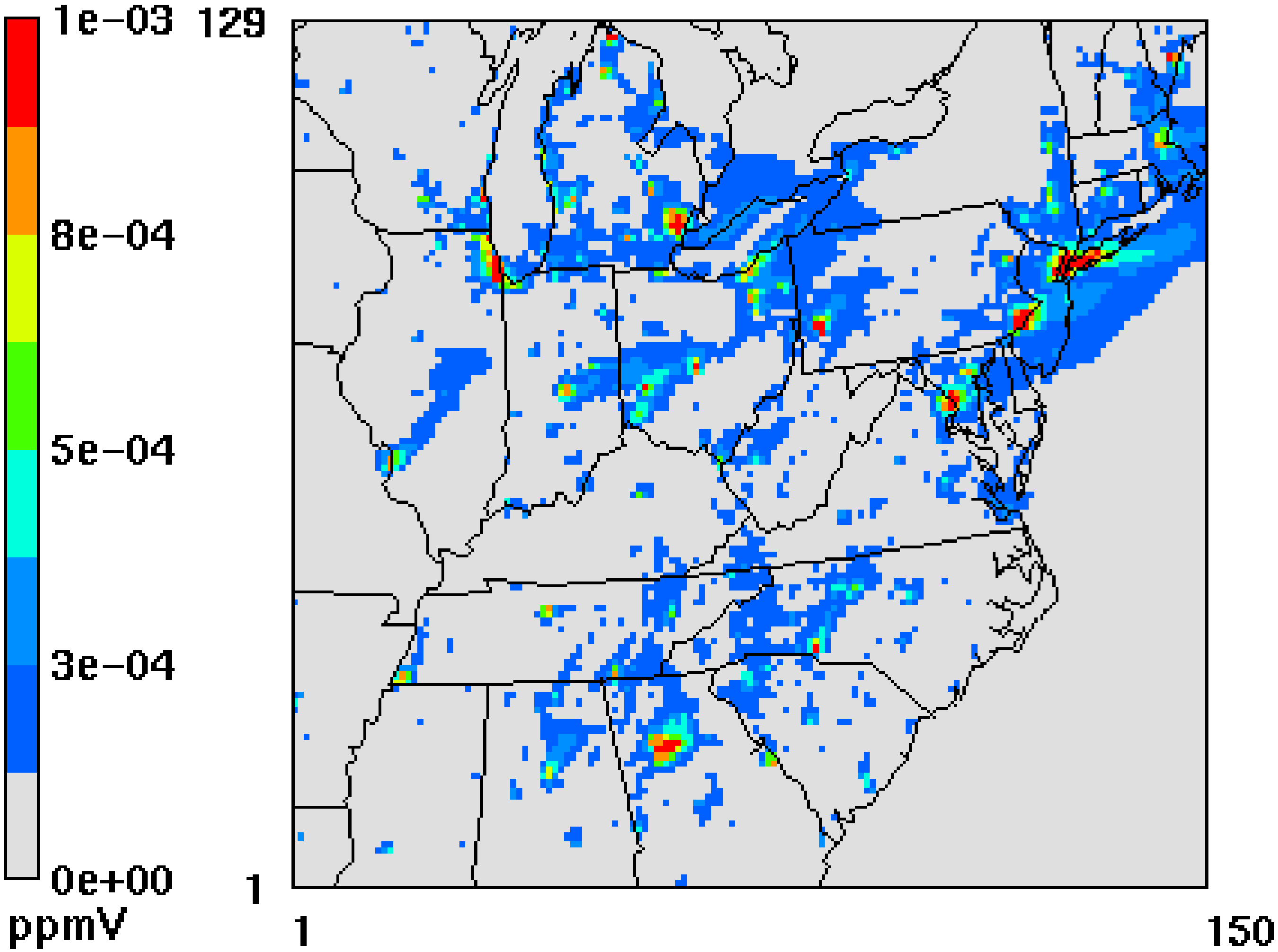
Regional pollutants (ozone, PM, mercury, etc.)

- These pollutants often result from interactions among pollutants released over broad regions over many days
- High concentrations depend on weather and air masses persisting for a few days
- Chemical reactions or particle formation depend on weather
- Removal by precipitation and dry deposition

Emissions of benzene over a broad region



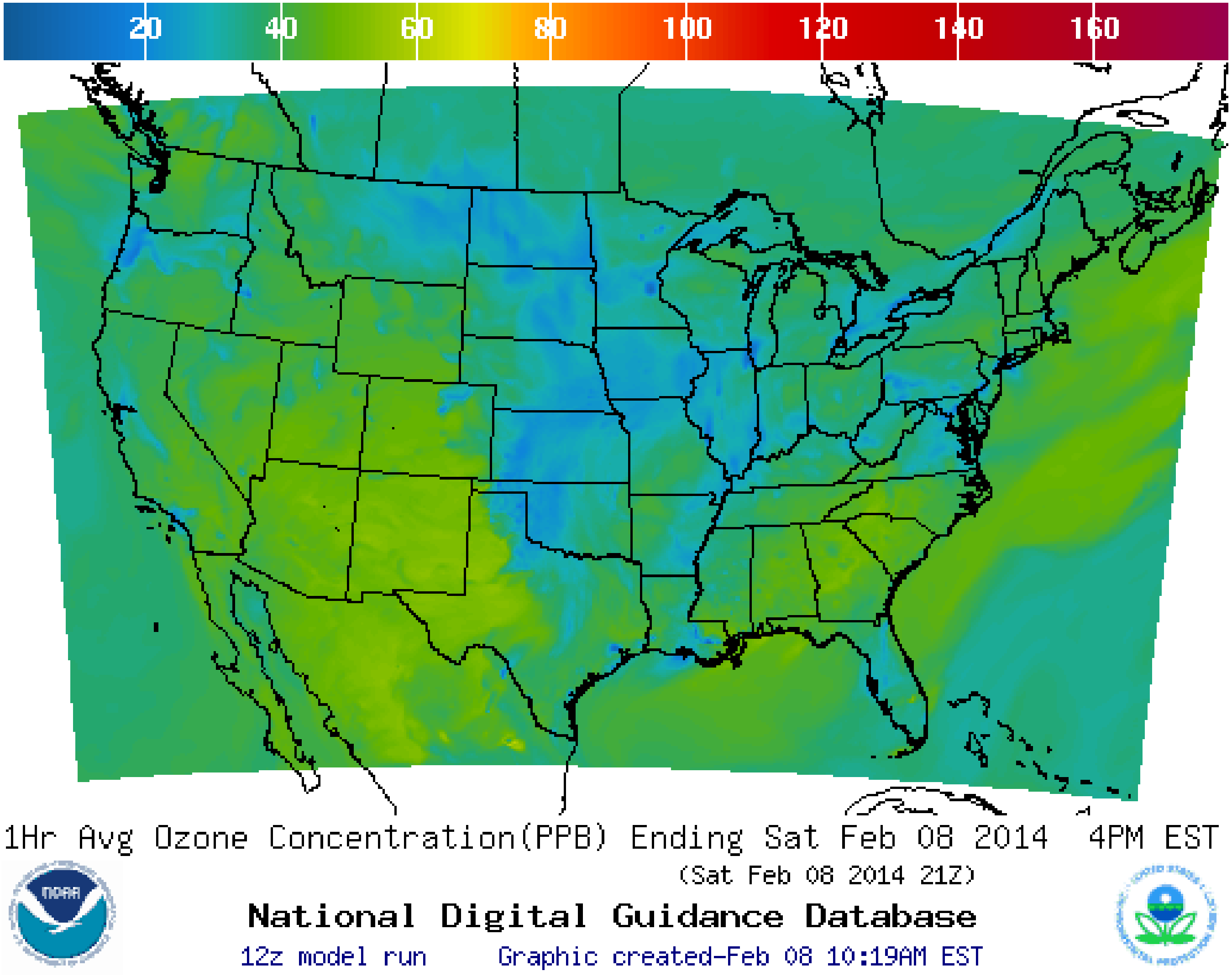
EPA's Community Multiscale Air Quality (CMAQ) model-predicted benzene concentrations (ppm) for the day with emissions shown on slide 15



Operational surface ozone forecast by NOAA NWS

(Uses WRF-CMAQ) airquality.weather.gov

NOAA web product – surface ozone ppb



Short-distance industrial plumes

- Maximum ground level impacts of, say, SO_2 or NO_2 or radiological pollutants occur within 10 km of the plant
- There is often a stack of elevation 50 m or more
- EPA requires modeling for permits; AERMOD is usually the T&D model
- Ground level impacts depend on wind speed, stability, and turbulence.
- Elevated plume may "hit" sides of hills.

Power Plant Plume Remaining Aloft during Stable Ambient Conditions

580 MW natural-gas-fired power generators. Note the short stacks. The plumes are very buoyant.

Mobile Sources - Cars, Trucks, Busses, Airplanes, Trains, Construction Equipment

- Multiple emissions sources (of CO, NOx, PM, VOC etc) are distributed over streets, highways, and broad areas
- All emissions are near ground and are estimated by approximations based on traffic density and speed
- There is a strong diurnal variation of emissions
- EPA has developed R-Line – a version of AERMOD, for application to traffic.
- Recent field experiments on effects of roadside barriers

Photo of Study Area Concerned with Local Impacts of Air Toxics at a U.S. Border Crossing: *Peace Bridge, Buffalo, NY*

Short time accidents (e.g., accident at industrial facility)

- Source emissions may be very uncertain
- Local weather conditions are needed
- Most important – conditions as close as possible to the location and time of the release (usually not available)
- Wind direction (carries plume to sensitive population)
- Stability and wind speed

Hyrocarbon release from refinery in Richmond, CA, August 2012. White cloud – prior to release catching fire. Black Cloud – after.

CFD (Computational Fluid Dynamics) T&D Models

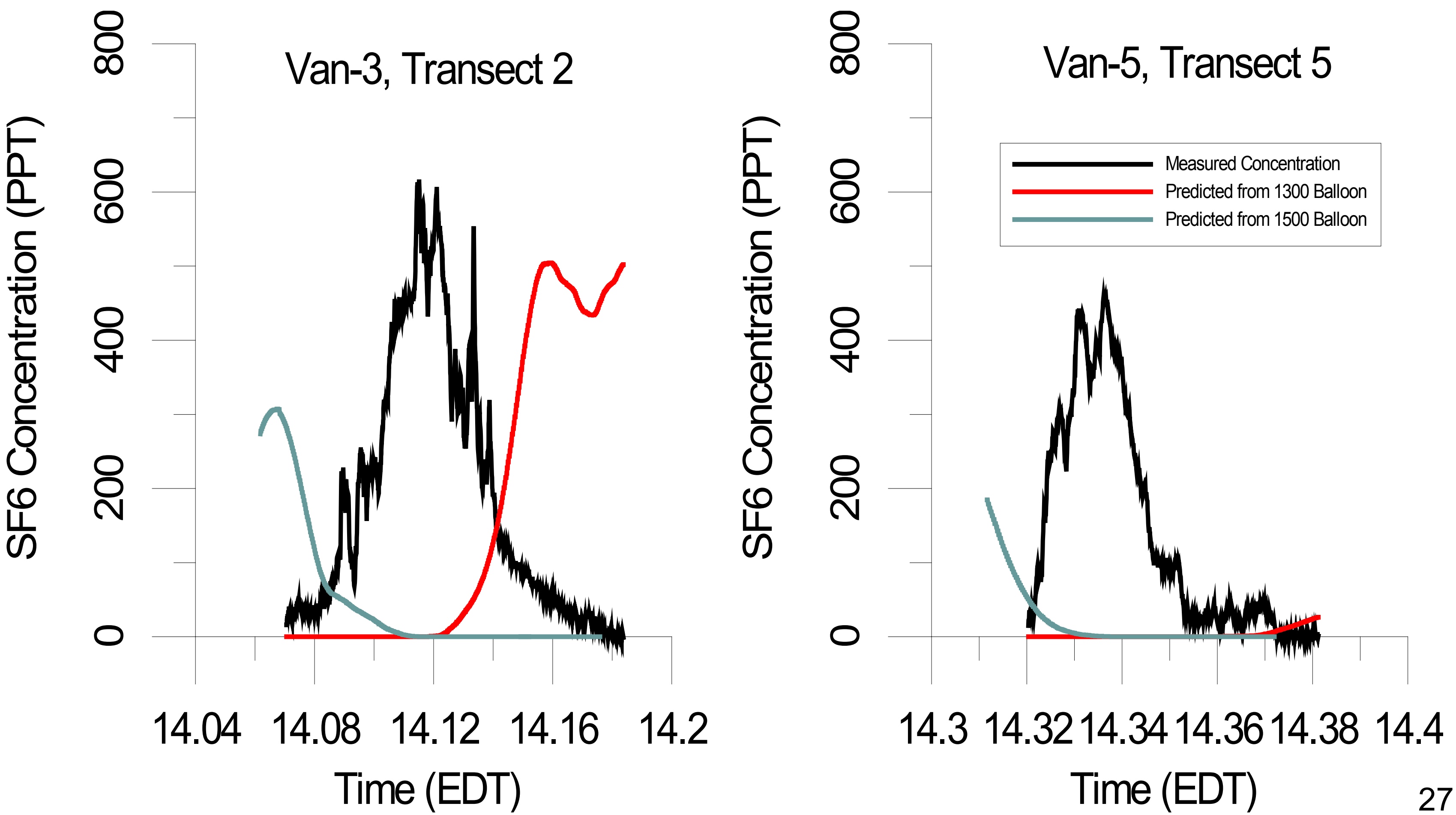
- Increasing use of CFD models for local studies, especially with significant terrain and obstacles (buildings, trees) (LES and RANS)
- They are found to give <u>precise</u> but not necessarily <u>accurate</u> predictions (see my comparison of five CFD models for Manhattan in the 2006 BAMS)
- e.g., AEOLUS (DOE-LLNL), FLUENT (commercial code), FLACS

Gaussian Plume Dispersion Models for Short Distances (Less than 50 km)

- (e.g., **AERMOD** used by **EPA** and **MACCS/ATMOS** by **NRC**) are based on the assumption of a Gaussian (normal) cross wind-distribution, with the standard deviations $\boldsymbol{\sigma_x}$ and $\boldsymbol{\sigma_y}$ and $\boldsymbol{\sigma_z}$ estimated based on theory and correlations with field experiments
- Straight line plume model for each hour
- **ATMOS** is actually a Gaussian slug model, which accounts for some variation in met inputs

Actual distributions are not exactly Gaussian

Tracer concentrations observed by a van 5 to 7 km from a tracer gas source at Cape Canaveral



Historical Gaussian Models for Plume T&D

In use from 1920s through present. Started with WWI, focused on chemical agent releases.

The Gaussian Plume model was used as a basis for many AEC and later NRC T&D models and in reg guides

The EPA Industrial Source Complex (**ISC**) model was widely used in the 1990s. In 2005, the EPA replaced **ISC** with a more scientifically-rigorous model, **AERMOD.** But AERMOD still usually assumes a Gaussian cross-wind distribution.

Straight-Line Gaussian Plume Model

- Assumes constant meteorological conditions for each hour, implying straight-line trajectories.

- Limited to source-receptor travel times and distances over which meteorological conditions are constant. But in operational use, the 50 km limit is the "rule of thumb".

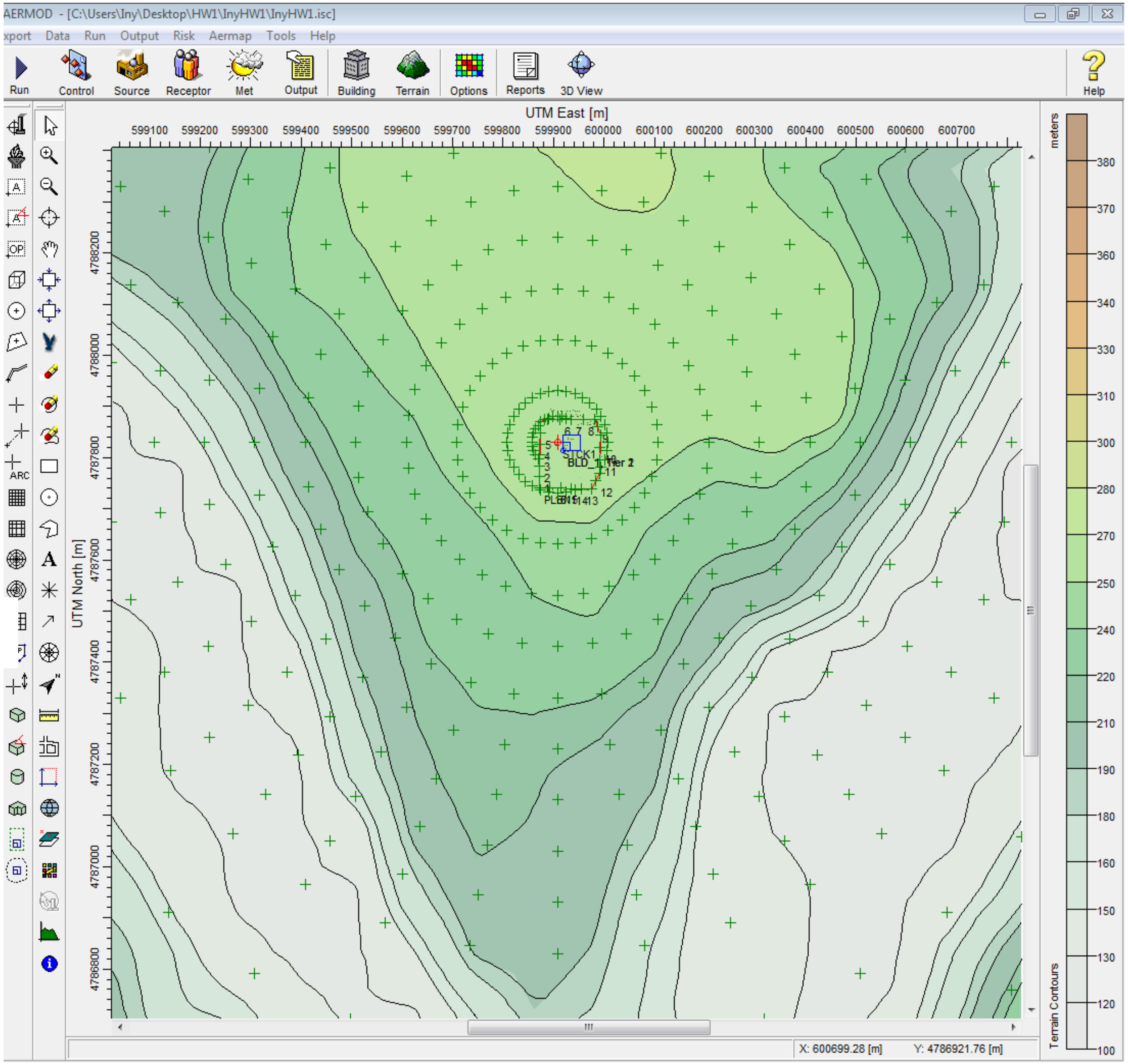
AERMOD

- The basic equations and logic are simple, but the regulations require calculations of impacts at many locations around the source for each hour for 5 years
- The model software spends most of its time on book-keeping outputs for the 43,800 hours and selecting max 24 hour concentration and other required statistics
- EPA model version is dos-based (old time code), but private companies sell versions with state-of-the-art GUIs
- MACCS/ATMOS saves computer time by defining 20 or 30 weather categories and assigning each hour in a year to that category. Then the model is run far fewer times.

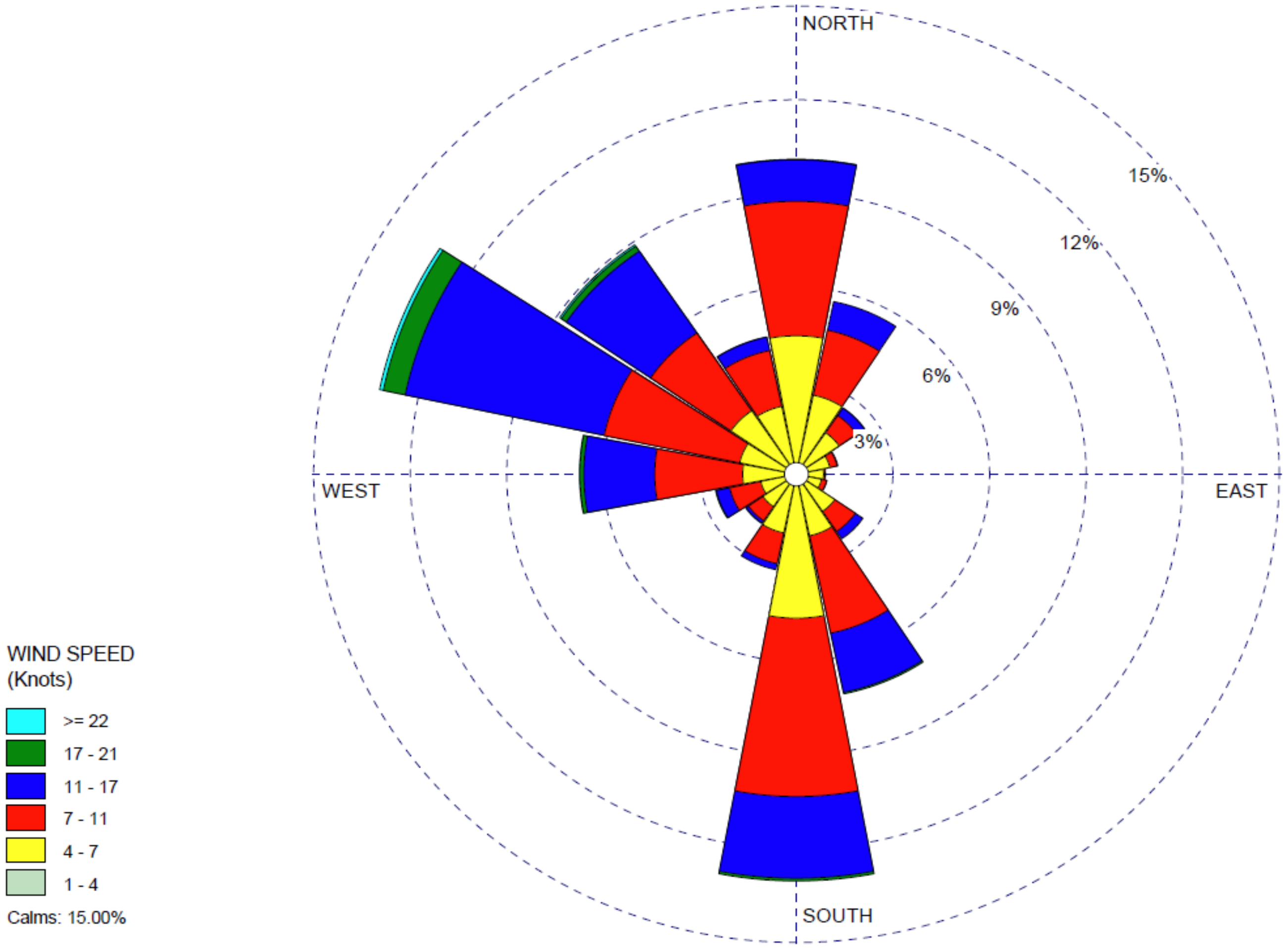
A few facts about AERMOD

- It uses high-resolution topography (terrain) data from USGS.
- It uses 1 to 5 years of hourly meteorological data from NOAA National Climatic Data Center.
- Software from vendors (e.g., Trinity, Lakes) will download the terrain and met data automatically.
- Designed by EPA to give consistent results
- Quick learning curve for new users

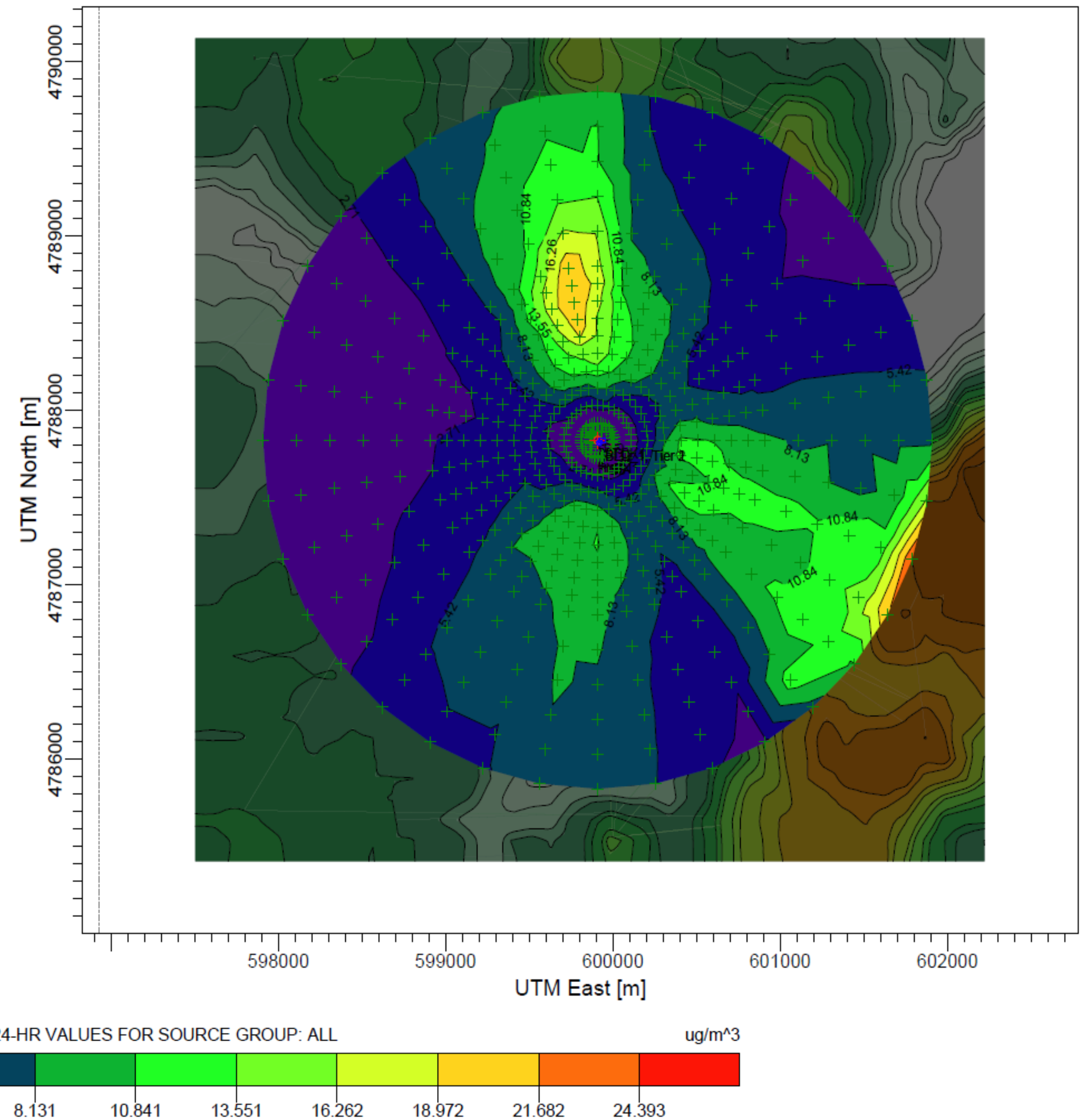
Example of plot of terrain contours generated by AERMOD software



Example of wind rose for airport surface observations for one year



Contour Plot of Highest Avg [SO_2] in 24 hrs for an AERMOD project



The high SO_2 on the edge is on a hillside

Dispersion Models for Moderate and Regional Distances

Lagrangian Puff Models – CALPUFF RATCHET, SCIPUFF

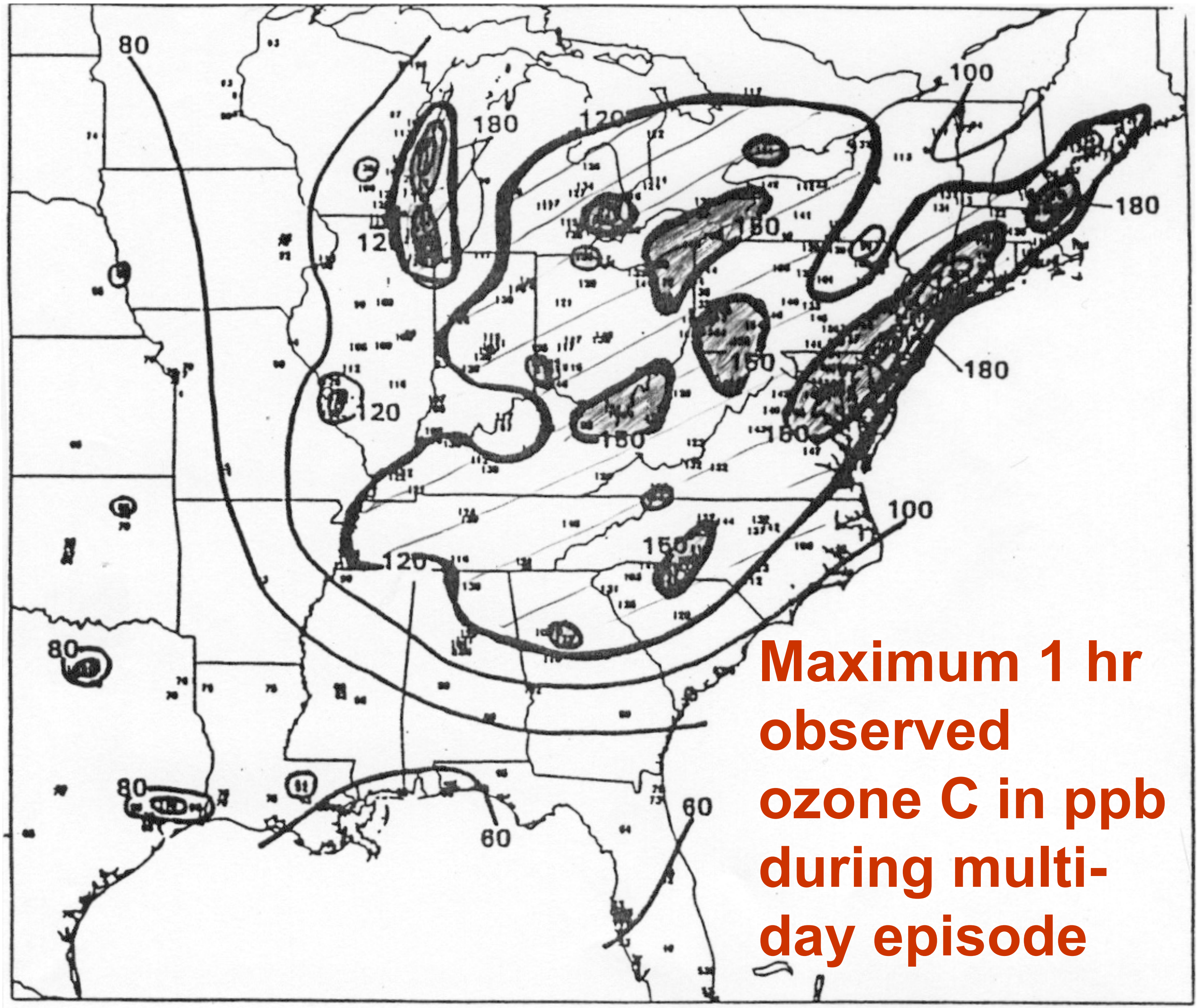
3-D Models - Focus on EPA's CMAQ

Hybrid - HYSPLIT

When to choose a puff model or a regional 3-D model

- A puff model (e.g., CALPUFF or SCIPUFF) is best for cases where the pollutant has limited chemical reactivity and the number of sources is <100 in a domain of size 20-200 km.
- A Regional 3-D model is best for cases where the pollutants are reactive and there are 100s or 1000s or more sources over a broad region (distances of hundreds of km)

Regional (not Local) Ozone Episode



Maximum 1 hr observed ozone C in ppb during multi-day episode

State-of-the-art Lagrangian Gaussian puff models

The term Lagrangian puff model means that the puffs move with the wind

e.g., the EPA's CALPUFF

or DTRA's HPAC/SCIPUFF or DOE's RATCHET

Lagrangian particle models are similar and are in use in many countries

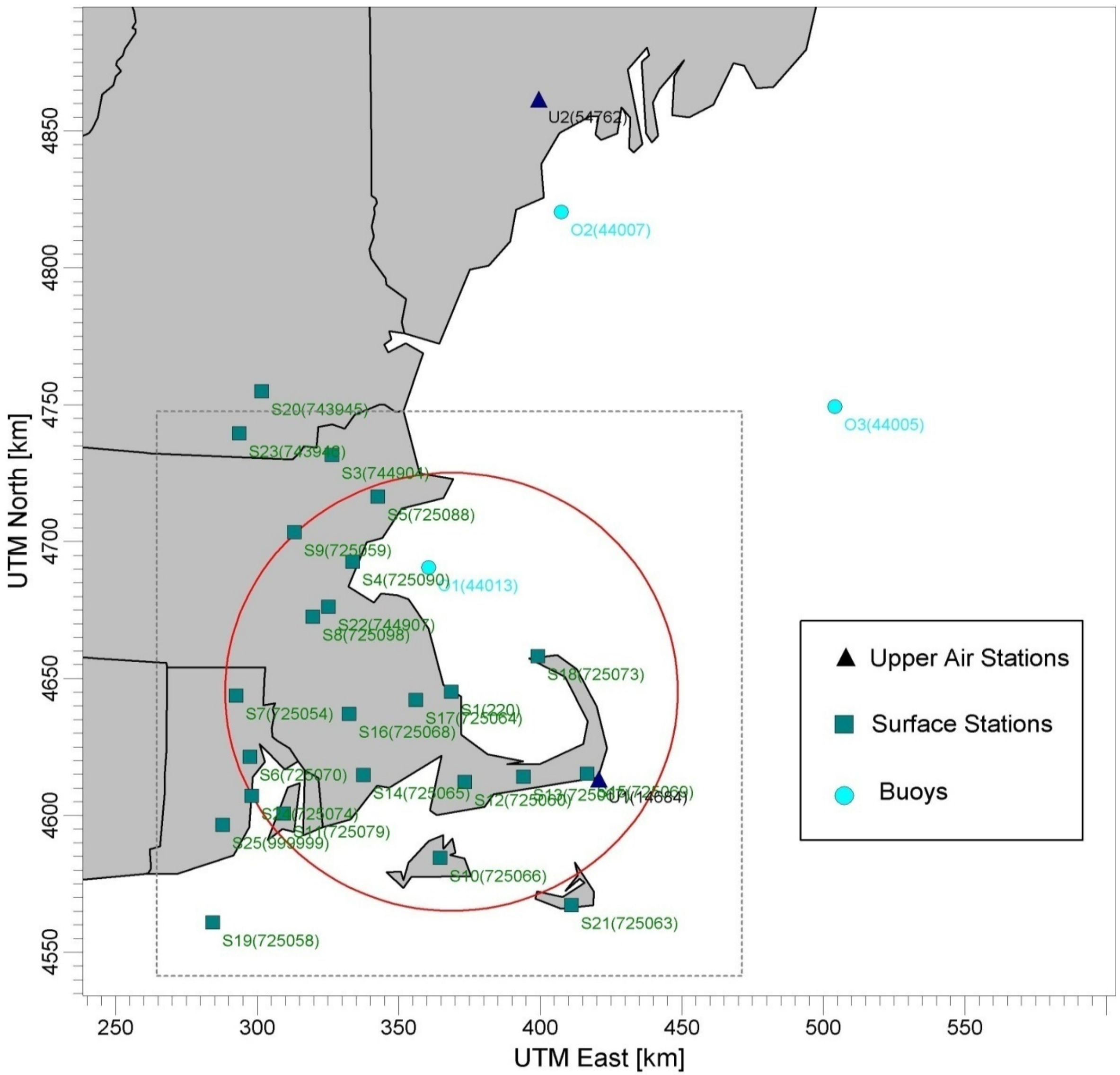
Differences among available US puff models

- **CALPUFF** is primarily for **EPA** applications and has a one-hour averaging time.
- **SCIPUFF** is used by many agencies and can handle instantaneous puffs
- **RATCHET** is used by DOE for radiological pollutants
- **HYSPLIT** is a hybrid LaGrangian Puff/Eulerian model run by **NOAA** and is for major national emergencies (e.g., volcanoes, large accidents, forest fires)

Advantages of puff models

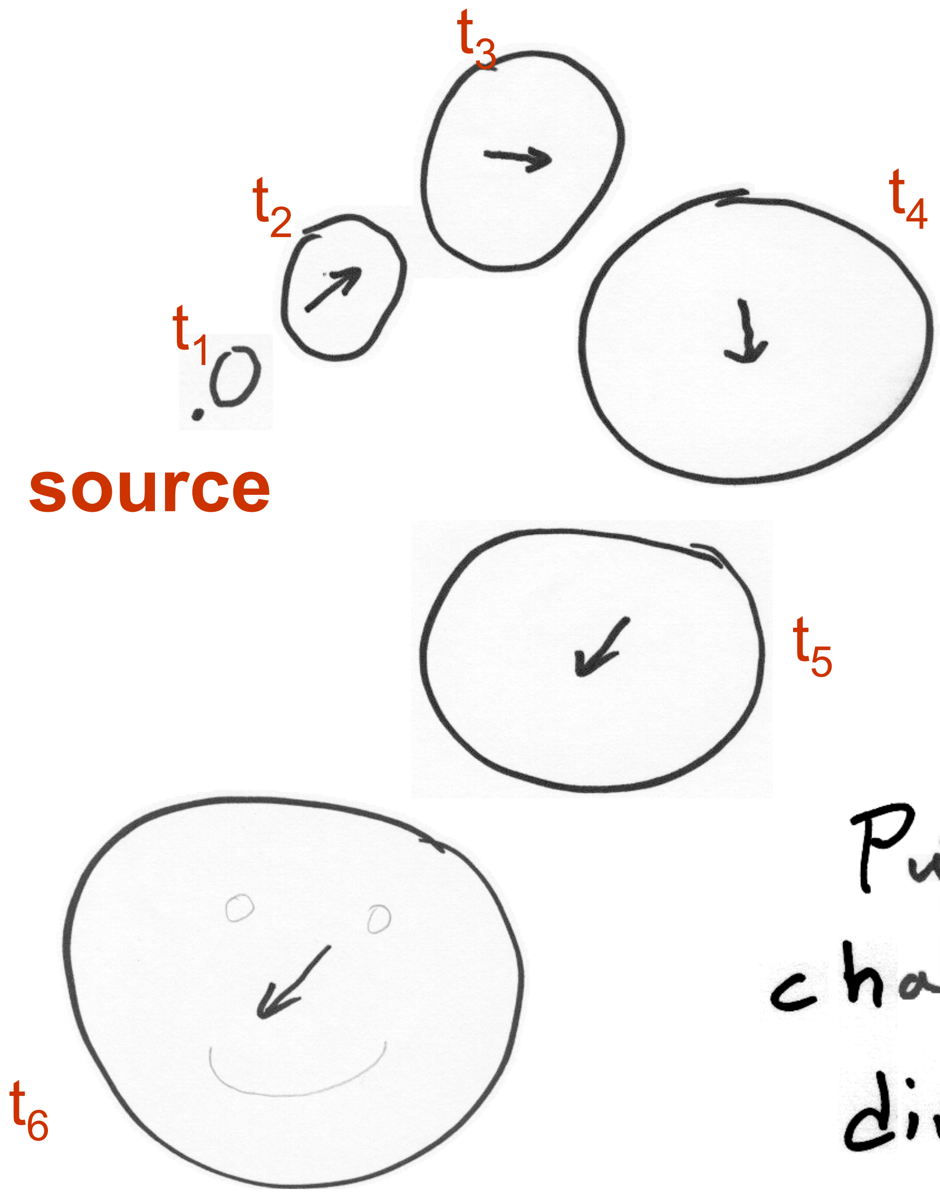
- The puff models overcome the objections to **AERMOD's** "straight-line, steady-state" assumption
- A puff model simulates a release over a period of time as a series of puff releases.
- Useful for distances of 20 to 200 km and times from one hour to two days.

Wind observing sites used for CALMET modeling of Pilgrim Station. Red circle is MACCS domain



All are official NOAA Sites with long term continuous records

Puff movement in a Lagrangian puff model



The arrow is the local wind vector

Puffs change direction

Puff transport and dispersion

- The center of the puff moves with the mean wind

$$\mathbf{x_2 = x_1 + u(t_2 - t_1)}$$

t_2 is new time and t_1 is previous time

- The dispersion (spread) of the puff at a new time $\mathbf{t_2}$ is expressed as, for example,

$$\boldsymbol{\sigma_y(t_2) = \sigma_y(t_1) + (t_2 - t_1)\sigma_v}$$

$\boldsymbol{\sigma_v}$ is turbulent velocity

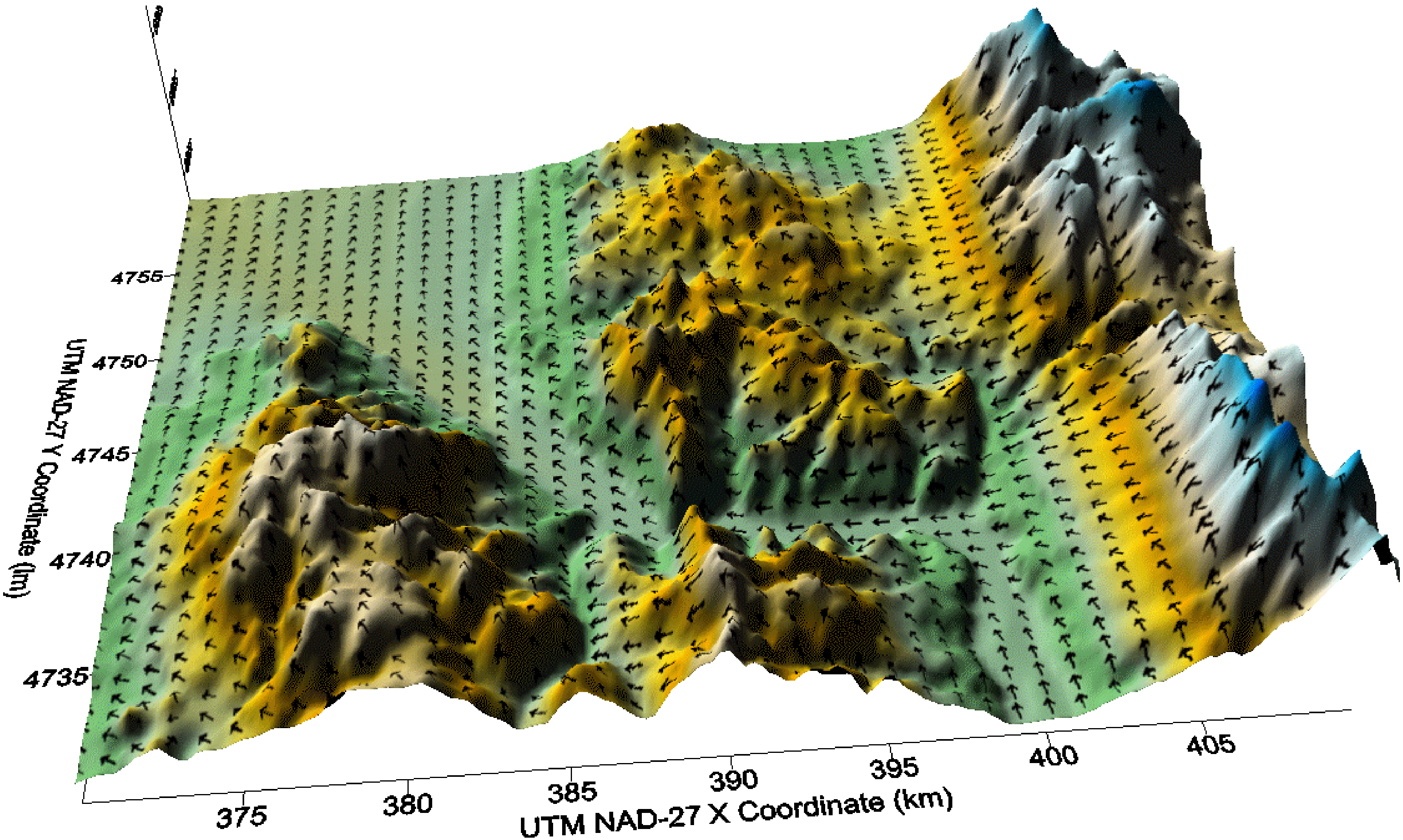
CALMET diagnostic wind model – Feeds winds to CALPUFF

Interpolate and extrapolate from wind observations at surface and aloft.

Apply mass-conservation constraint to adjust winds.

Can account some for wind turning due to terrain

CALMET wind vectors on 3-D terrain map (near Salt Lake City)



National Weather Service (NWS) weather forecast models

- Solutions to fundamental equations
- Horizontal grid size of about 10 km and vertical grid size of about 10 m next to ground and 200 m at top of mixed layer
- Can be run in forecast mode or in historical reconstruction mode
- Produce large amounts of output that must be processed for input to **CALPUFF** or **SCIPUFF** or other models
- **Weather Research Forum (WRF)** model
- Note – All agencies are moving towards use of these forecast wind models