An ATD Model that Incorporates Uncertainty

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Methods for Estimating Uncertainty

a) Explicit methods
   - compute a representative collection of possible results, e.g.
     i. Monte Carlo
     ii. Large Eddy Simulation
   - *generally straightforward, but computationally expensive*

b) Statistical Methods
   - compute statistics directly, e.g.
     i. PDF
     ii. Statistical moments
   - *generally computationally efficient, but difficult to formulate*

SCIPUFF ATD Model

- SCIPUFF uses simplest statistical method
  - develop conservation equation for first two moments
  - i.e., concentration mean and fluctuation variance
  - use simple 2-parameter pdf to estimate probability
  - implement in Lagrangian puff model

- Start with scalar diffusion equation

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}\left(u_i\, c\right) = \kappa \frac{\partial^2 c}{\partial x_i\, \partial x_i}$$

  - where $\boldsymbol{u}$ is the turbulent (random) velocity

Ensemble Statistics

- Define ensemble average
  - not trivial in unsteady, inhomogeneous atmosphere

- Use classical techniques to develop equations for mean, $\overline{c}$, and variance, $\overline{c'^2}$

- Turbulent concentration fluctuations
  - driven by velocity fluctuations
  - determined largely by dissipation rate
  - modeled in terms of turbulence spectrum

Sources of Uncertainty

- Meteorology
  - wind field
    - turbulent boundary layer fluctuations
    - mesoscale fluctuations
    - uncertainty (forecast or analysis/interpolation)
  - thermodynamics
    - temperature
    - humidity
  - boundary layer
    - stability
    - mixed layer depth
    - turbulence intensity

More Sources of Uncertainty

- Landcover
    - roughness / canopy
    - terrain
- Physical processes
    - liquids
        - liquid droplet/pool evaporation
        - liquid absorption / desorption
    - particles
        - gravitational settling
        - dry deposition
- Source characteristics, etc., etc.

SCIPUFF Uncertainty

- Generally limited to windfield
  - expected to be significant and irreducible
  - can also describe source location uncertainty via initial conditions
- Need estimates for
  - turbulence intensity, $\overline{u'^2}, \overline{v'^2}$, etc.
  - turbulence correlation scales, Λ
- Boundary layer turbulence (reasonably) well understood
  - idealized shear- and buoyancy-driven layers
  - investigating use of mesoscale model TKE for more general cases
- Mesoscale and Forecast Uncertainty poorly understood

Large Scale Variations

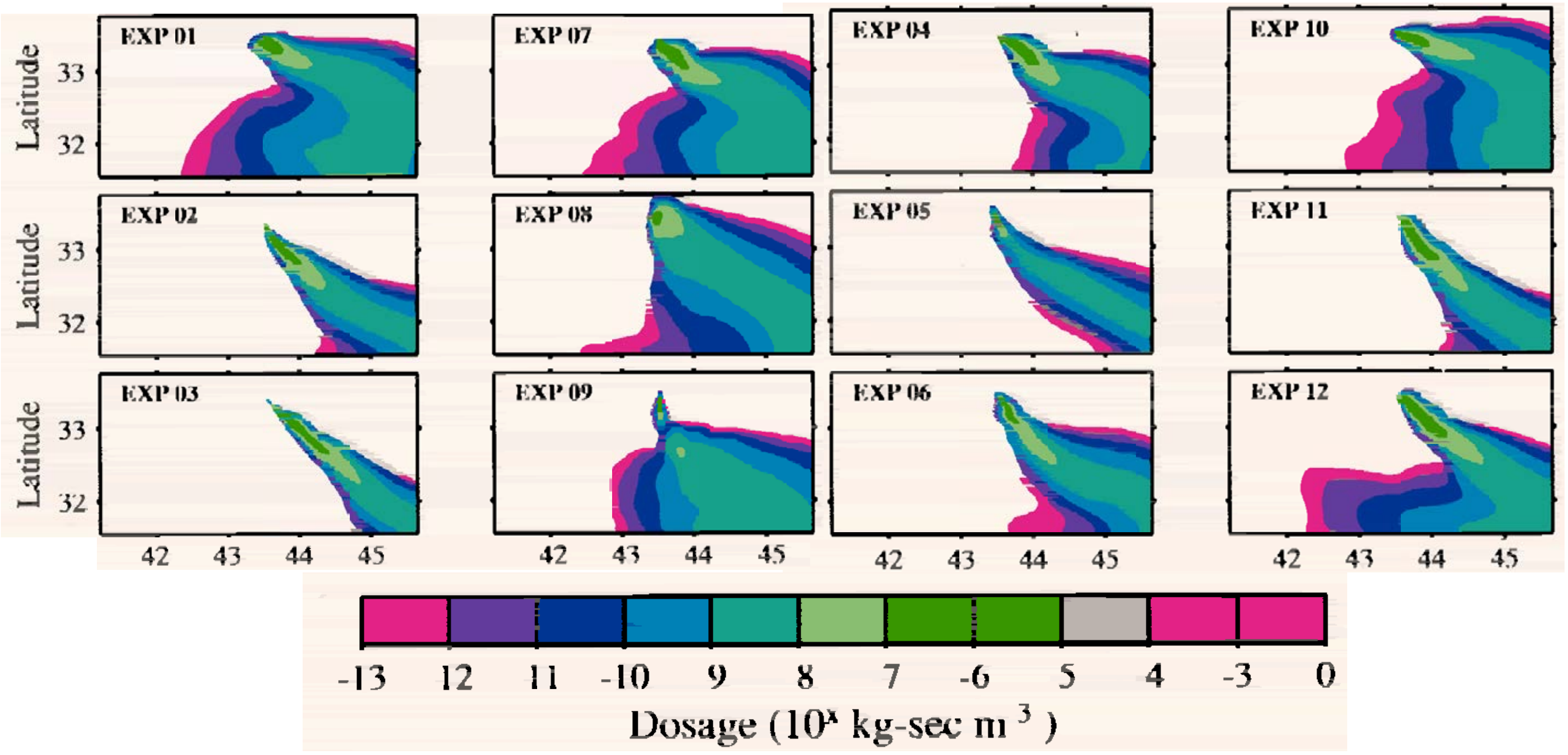
- Large Scale means larger than PBL scale
  - important for assessing long range dispersion
  - also required for forecast/analysis uncertainty
- Ensemble forecasts
  - explicit calculation of an ensemble provides a direct measure of velocity statistics
  - limited sample gives velocity variances
  - may be able to estimate Lagrangian autocorrelation timescale
- Subgrid fluctuations
  - depends on subgrid terrain / landcover
  - energy cascade from larger scales
  - Smagorinsky model unlikely to be adequate for dispersion

Role of Ensemble Modeling

- Ensemble methodology is generally applicable
  - can describe any quantifiable uncertainty
  - requires explicit description of random distribution of input / model parameters
  - relatively expensive
  - difficult to ensure complete coverage of all possible conditions
- Combined ensemble / statistical approach
  - use statistical techniques to model limited range of uncertainty within larger ensemble
  - e.g. use SCIPUFF to represent range of conditions within a set of sub-ensembles

MM5 Dispersion Ensemble

Warner et al (JAM, 2002)



Ensemble Statistics

- One-point correlations are straightforward
  - mean: $\overline{u} = \dfrac{1}{N}\sum_{i=1}^{N} u_i$
  - variance:

$$\overline{u'^2} = \frac{1}{N}\sum_{i=1}^{N}\left(u_i - \overline{u}\right)^2, \quad \overline{u'v'} = \frac{1}{N}\sum_{i=1}^{N}\left(u_i - \overline{u}\right)\left(v_i - \overline{v}\right), \quad etc.$$

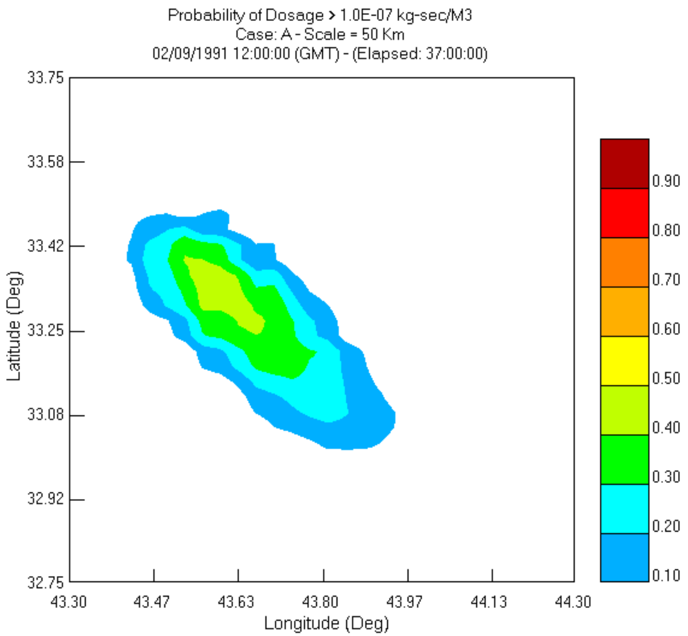
- Length / Time Correlation scale is more difficult
  - investigate Lagrangian autocorrelation

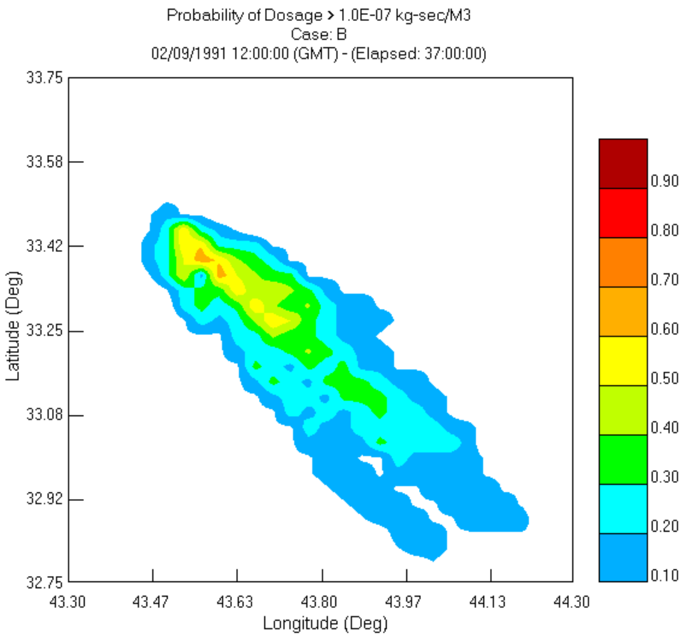
$$R_{uu}\left(\tau; \boldsymbol{x}_0, t_0\right) = \frac{\dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\overline{u_i'\left(\boldsymbol{x}_0, t_0\right)u_i'\left(\boldsymbol{x}_{\boldsymbol{i}}\left(\tau\right), t_0 + \tau\right)}}{\sigma_u\left(0\right)\ \sigma_u\left(\tau\right)}, \quad \text{and} \quad \frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{u}_i$$

Probability of exceeding 10^{-7}kg-s/m^3

SCIPUFF Statistical Prediction

MM5 Explicit Ensemble





Concluding Remarks

- Many sources of uncertainty in atmospheric dispersion predictions
  - sensitivity studies are needed to quantify/prioritize other uncertainties
- Meteorological uncertainty is known to be important
  - ensemble modeling promises characterization of large (resolved) scale uncertainty
  - subgrid mesoscale/synoptic requires research
- SCIPUFF modeling approach
  - provides an efficient treatment of a major component of uncertainty
  - can be combined with explicit approaches for more generality