DEFENSE THREAT REDUCTION AGENCY

DTRA
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CHEMICAL/BIOLOGICAL SOURCE CHARACTERIZATION

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S&T CBIS, October 25-28, 2005

OUTLINE

- Background
- Problem
- Previous Work
- Proposed Solutions

BACKGROUND

- Atmospheric Transport and Dispersion (ATD) Models
- Puff or Plume Models
- Estimate Location and Population Affected
- Key Elements
  - Size and Location of Release
  - Meteorological Data

PROBLEM

- Accidental or Terrorist Release
  - Source is Unknown (Size and Location)

- Therefore Hazard Prediction is Poor

- Identification of Source is Critical

PREVIOUS WORK

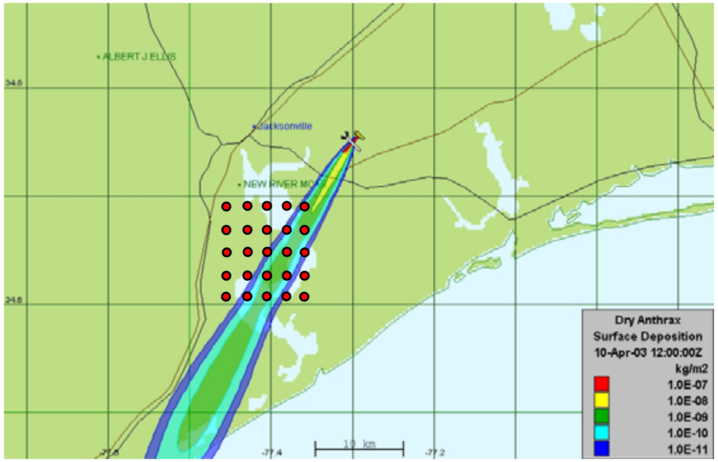
- Fundamental Question for Environmental Science
  - Pollution Source Attribution
- Accidental Release
  - Chemical or Nuclear Plant or Transportation Accident
- Solution
  - Large Sensor Grid
  - Use ATD and Limited Sensor Data

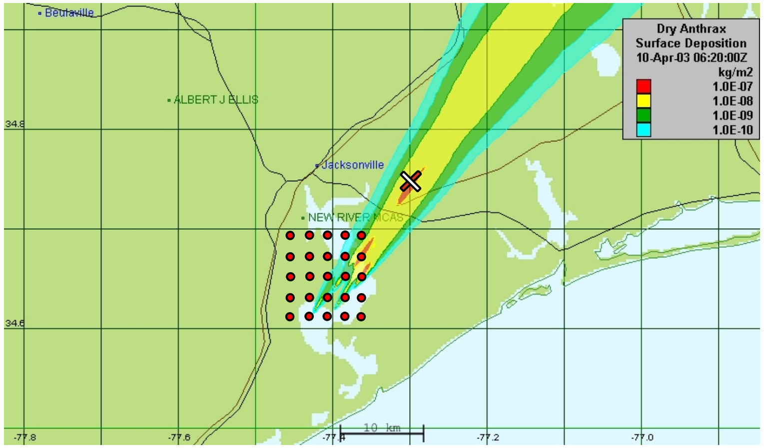
PROPOSED SOLUTIONS

- FORWARD
  - Guess Source
  - Use ATD to Estimate the Hazard
  - Does it Match?
  - Iterate Guess and Recalculate
  - Lots of Runs Required
- BACKWARD
  - Reverse Time
  - Use Sensor Data and Run ATD Backward
  - NOT THAT SIMPLE

BACKWARD METHODS

- Adjoint Transport
- Reverse Diffusion





ADJOINT TRANSPORT

- Concept of Reverse Diffusion is based on the Adjoint Model
- Adjoint provides "inverse" relation between model input (release parameters) and output (sensor measurement)
- Inverse applies for a general class of sensors

ADJOINT TRANSPORT OPERATOR

- For the advection-diffusion equation

$$L(c) = \frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i c) - \kappa \nabla^2 c$$

we have

$$L^*(c^*) = -\frac{\partial c^*}{\partial t} - u_i \frac{\partial c^*}{\partial x_i} - \kappa \nabla^2 c^*$$

which can be interpreted as reverse time, reverse velocity, but positive diffusion

GENERAL SENSOR

- KEY TO THE METHOD – Mapping Sensor Response Back to a Source
- Assume sensor output can be expressed as a linear function (weighted integral) of the concentration field

$$S = \int c(\mathbf{x},t) R^*(\mathbf{x},t)\, d^3\mathbf{x}\, dt = \langle c, R^* \rangle$$

where R^* is the sensor response function

  – example is point sensor at $\mathbf{x}_0$, t_0 : $R^* = \delta(\mathbf{x}-\mathbf{x}_0, t-t_0)$

- Solve Adjoint System: $L^*(c^*) = R^*(\mathbf{x},t)$

- Adjoint Concentration gives Relationship between Source and Sensor Output

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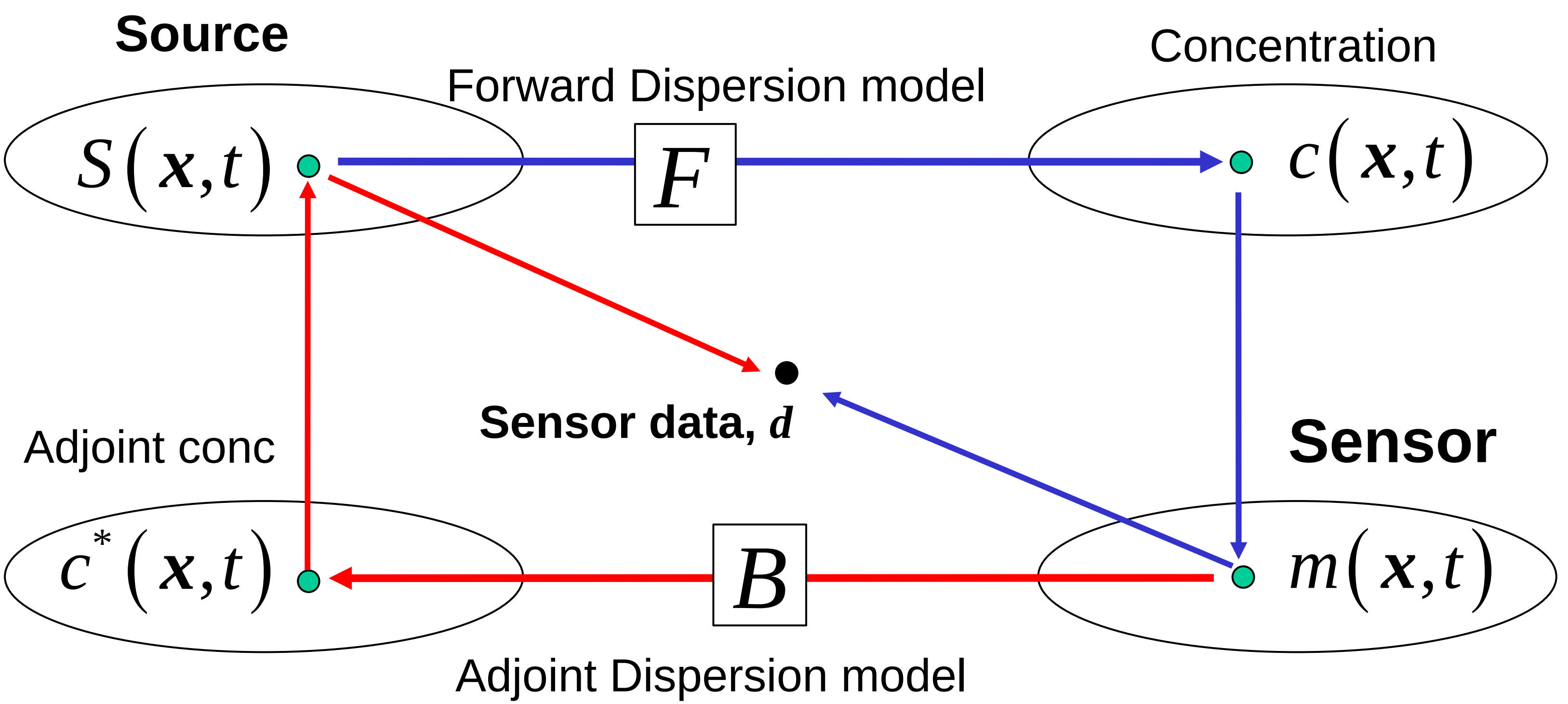
ILLUSTRATED SCHEMATICALLY



MULTIPLE SENSORS

- Any sensor data, *S*, defines a complete field (upwind space and previous time) of release mass, *Q*, "possibilities"

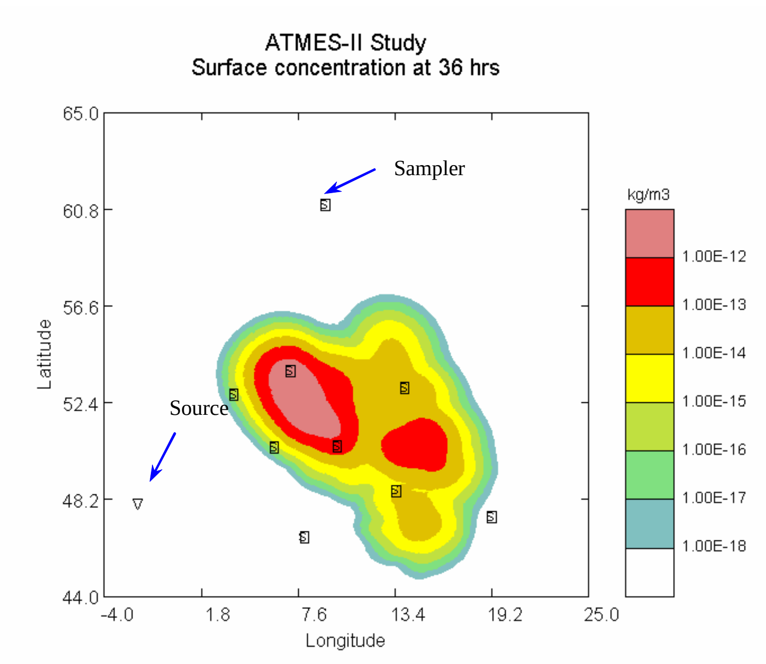
- Use multiple sensors to determine locations of consistency, i.e., same release mass for all sensors

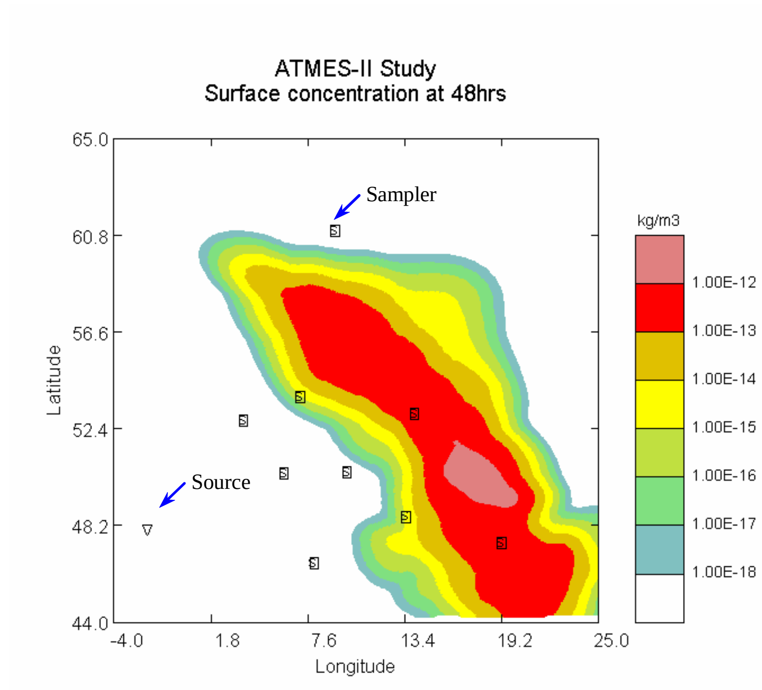
- Note this requires a separate reverse calculation for each sensor measurement

- Release location function
  - need a measure of the range of estimates
  - wider range implies less likely as a release estimate

IDEALIZED CASE

- Use HPAC to generate sensor data for a 4100kg release over 1 hour using ETEX meteorology





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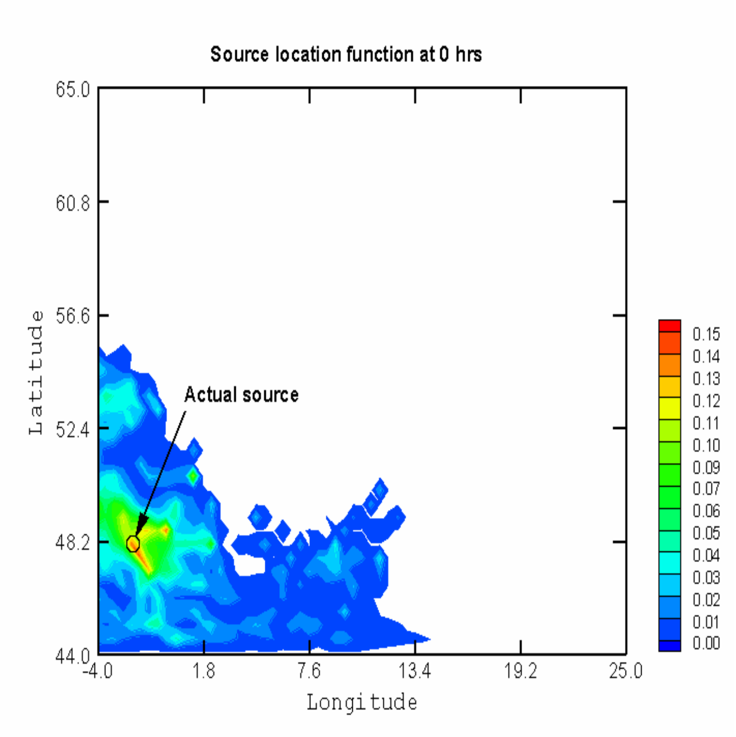
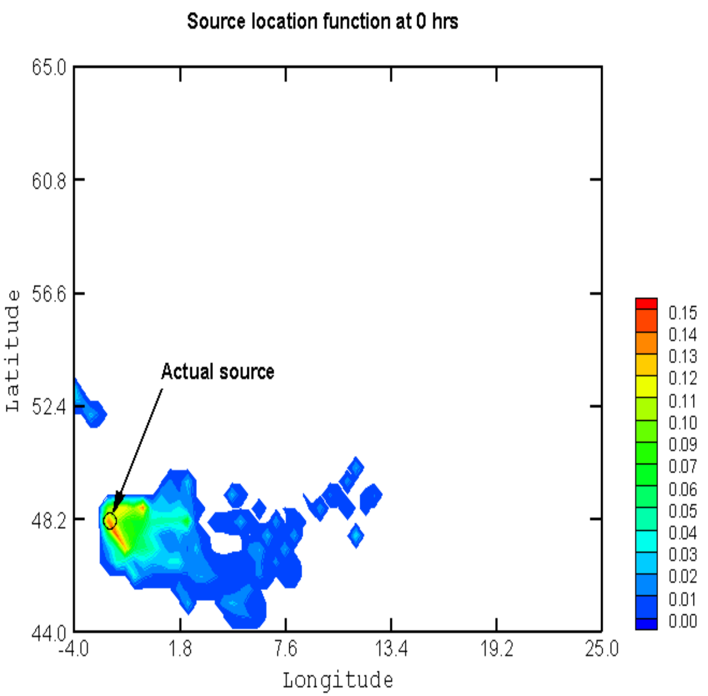
RELEASE ESTIMATE

- Release Location Function without/with Null data
  - release mass estimate is 2400kg





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TANGENT LINEAR ADJOINT

- Utilizes Automated Differentiation
- Uses Cost Function, *J*
- Jacobian of Transport Function

$$\frac{\partial J(\boldsymbol{y}(\boldsymbol{x}))}{\partial x_i} = \sum_k \frac{\partial F_k}{\partial x_i} \frac{\partial J}{\partial y_k}$$

or $$\nabla_x J(\boldsymbol{y}) = K^T \nabla_y J(\boldsymbol{y})$$

- Refines Initial Source Estimate
- Refines Hazard Prediction

FUTURE WORK

- Generalize sensor and release types

- Investigate probabilistic aspects
  - can we reverse the fluctuation variance equation?

- Investigate Bayesian or other techniques for combining sensor and other data
  - improved definition of source location/strength probabilities
  - multiple source possibility

SUMMARY

- Will Provide Statistical Estimate of Source
  - Location and Strength
  - Improved Estimate of Effective Area and Population

- Proven Science that will provide an Answer