HYSPLIT inverse modeling - Investigation using Cross Appalachian Tracer Experiment (CAPTEX) data and ensemble dispersion simulations

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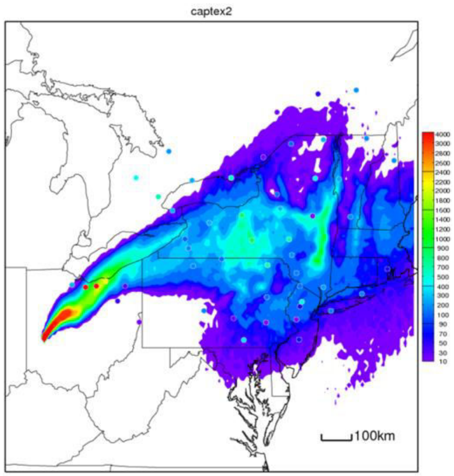
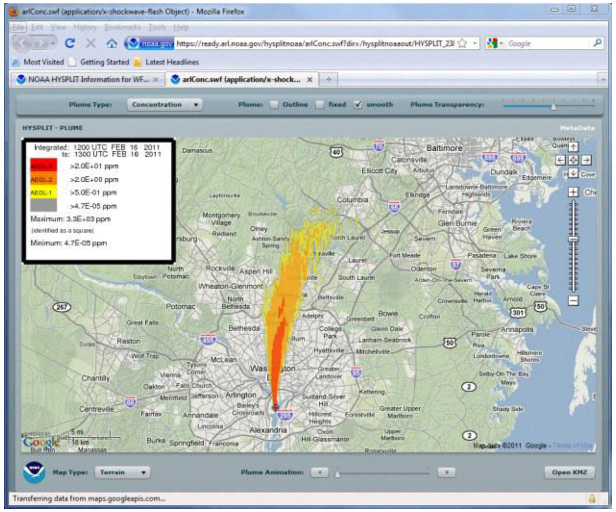
HYSPLIT model

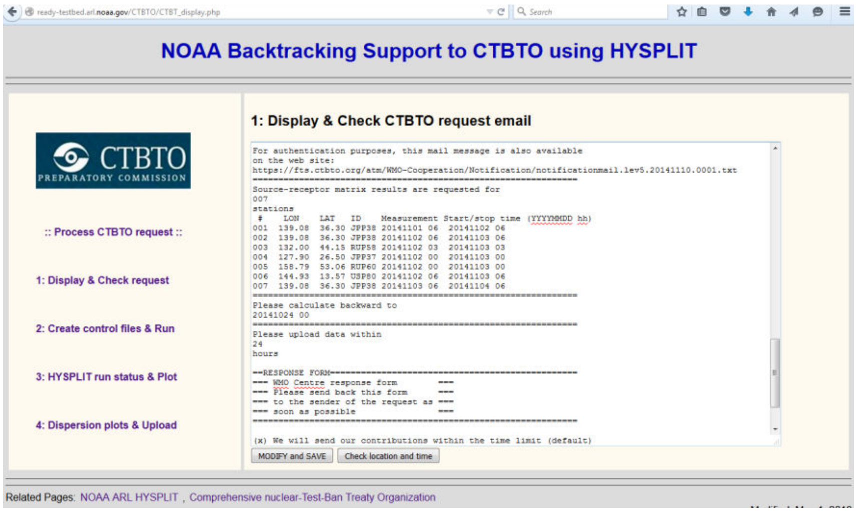
- HYSPLIT allows Lagrangian representations of the transported air masses w/ 3D particles, puffs, or a hybrid
- Applications include the simulation of atmospheric tracer release experiments, radionuclides, smoke originated from wild fires, volcanic ash, mercury, and wind-blown dust, etc.

CAPTEX



Emergency Response Chemical Releases



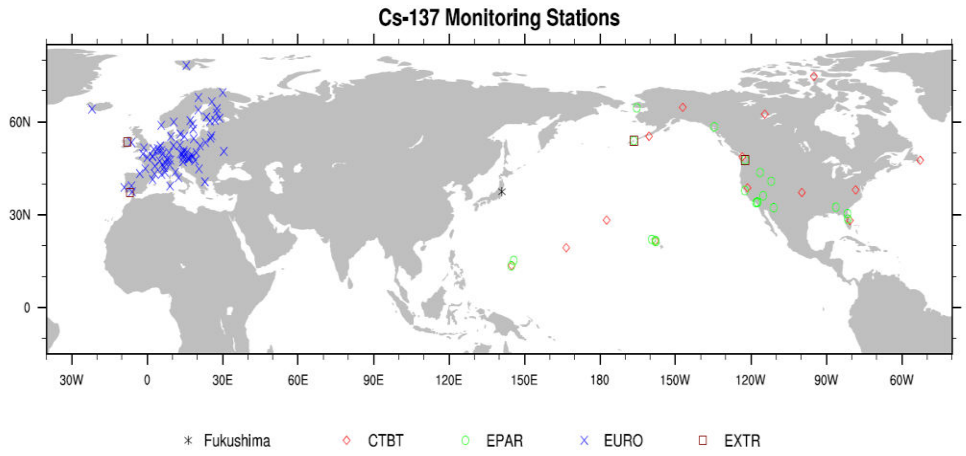


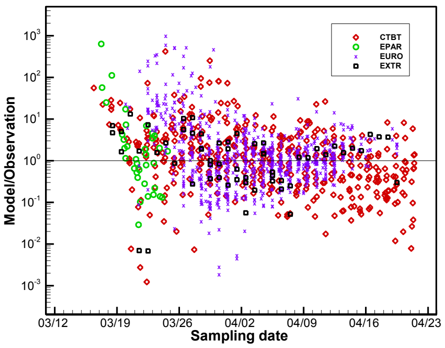
HYSPLIT Inverse Modeling

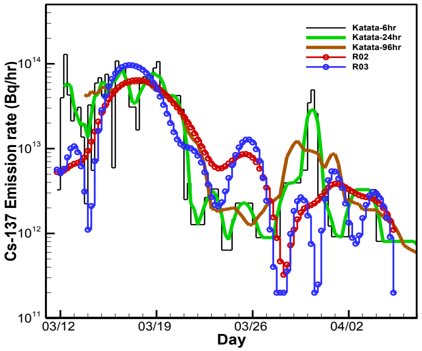
A general data assimilation approach: minimizing a cost function that mainly measures the differences between observations and predictions, for the entire time period and 3-D computational domain (4D-Var)

$$\mathcal{F} = \frac{1}{2}\sum_{n=1}^{N}\frac{(q_n - q_n^b)^2}{\sigma_n^2} + \frac{1}{2}\sum_{m=1}^{M}\frac{(c_m^h - c_m^o)^2}{\epsilon_m^2}$$

$$+ \; c_{sm}\cdot\sum_{n=2}^{N-1}\frac{1}{2}\left[\frac{(q_{n-1} - q_{n-1}^b) - 2\cdot(q_n - q_n^b) + (q_{n+1} - q_{n+1}^b)}{q_c}\right]^2$$



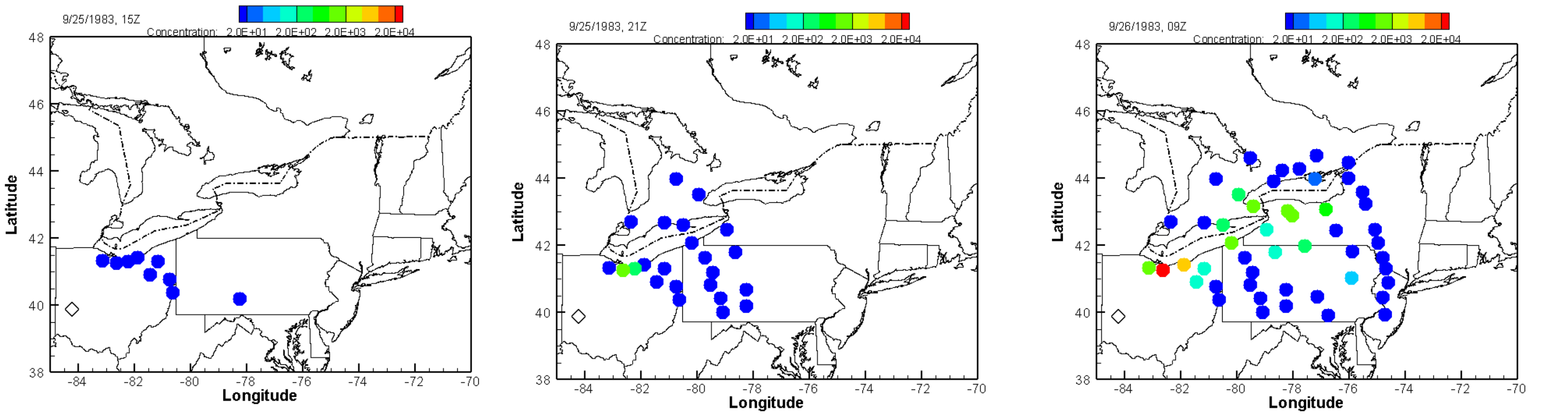




Source term estimation using air concentration measurements and Lagrangian dispersion model – Experiments with pseudo and real cesium-137 observations from the Fukushima nuclear accident, Chai, T., R. R. Draxler, and A. Stein, *Atmospheric Environment,* 106, pp. 241-251

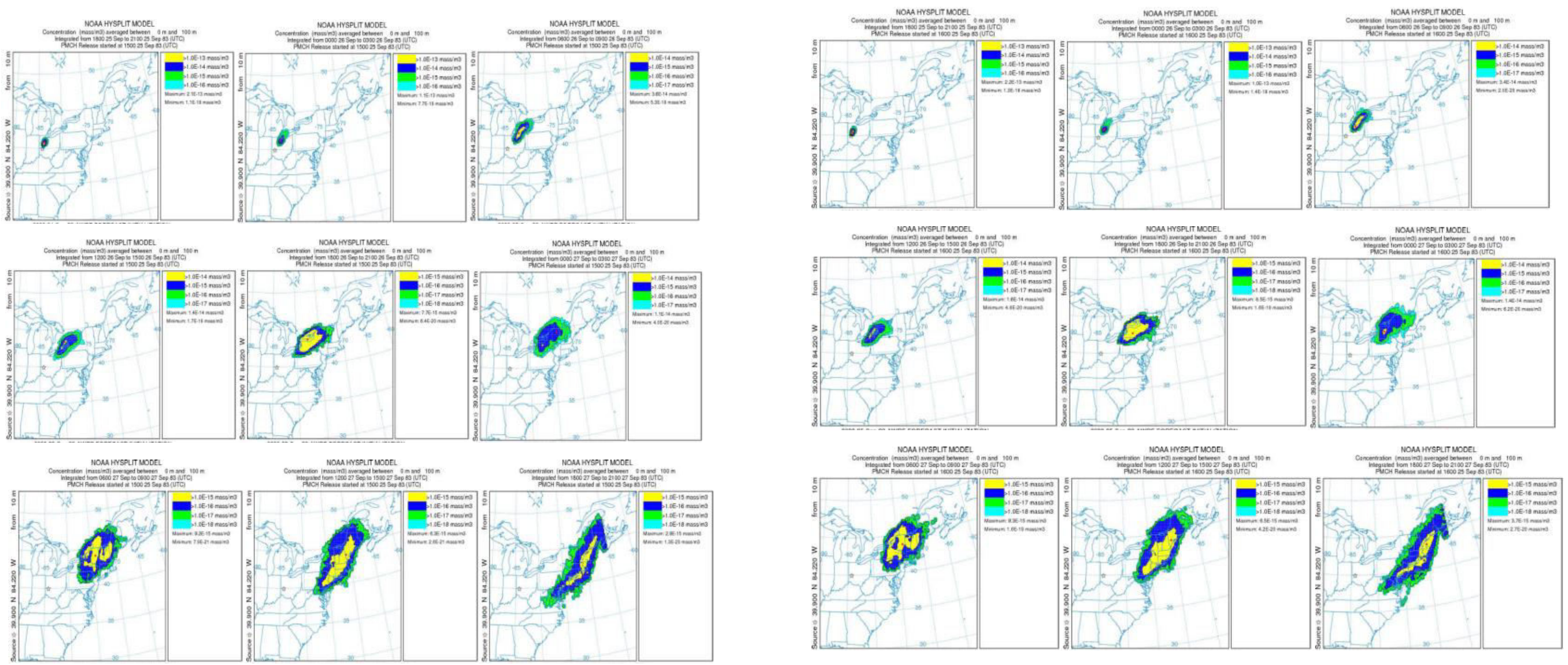
Cross Appalachian Tracer Experiment (CAPTEX)

- It consisted of a near-surface release of the inert tracer perfluro-monomethylcyclohexane (PMCH).
- Release 2 started at 17Z on Sep. 25, 1983, from Dayton, Ohio, USA.
- Samples were collected at 84 different measurement sites distributed from 300 to 800 km downwind of the emission source, as either 3- or 6-hour averages up to 60 hours after each release.



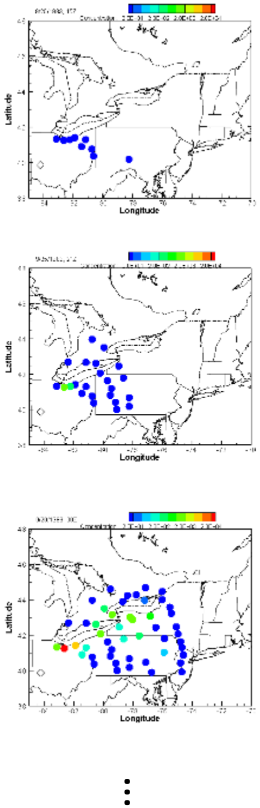
Forward-based inverse modeling

- Formulate the problem: Which part(s) of the release (strength, location, and temporal variations) need(s) to be solved
- Simply the problem by having a limited number of unknowns: For instance, the emission vary hourly or 3-hourly
- Run each release candidate with unit emission and get transfer coefficient at all observation point

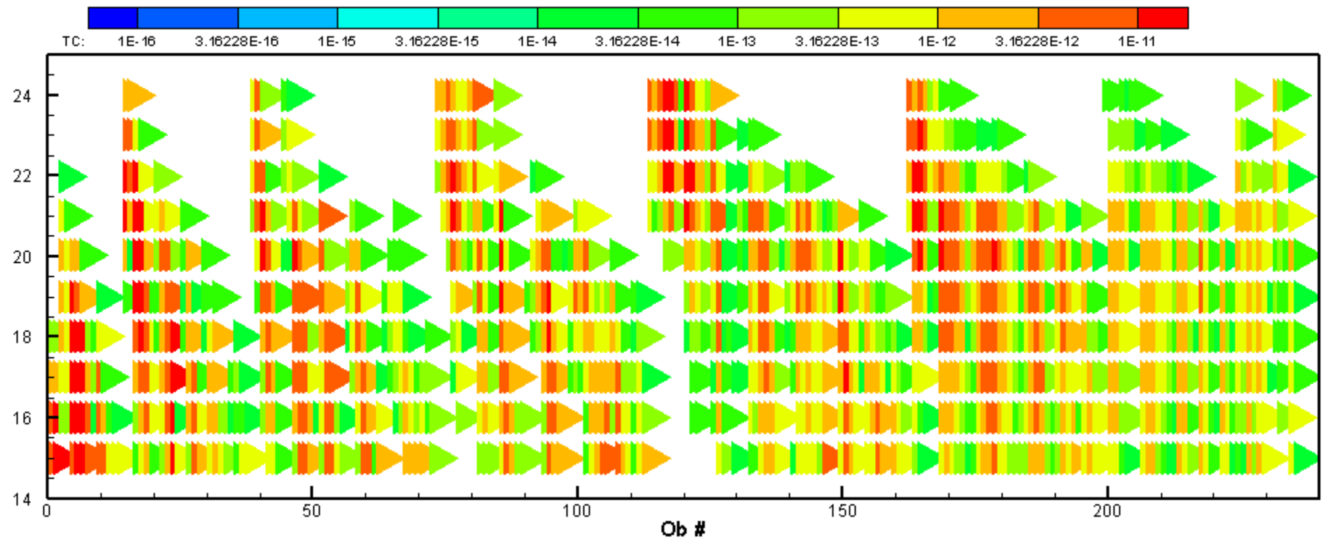


HYSPLIT simulations with unit emission from Dayton Ohio, started at 15Z (left) and 16Z (right) on September 25, 1983.

Transfer coefficient matrix (TCM)

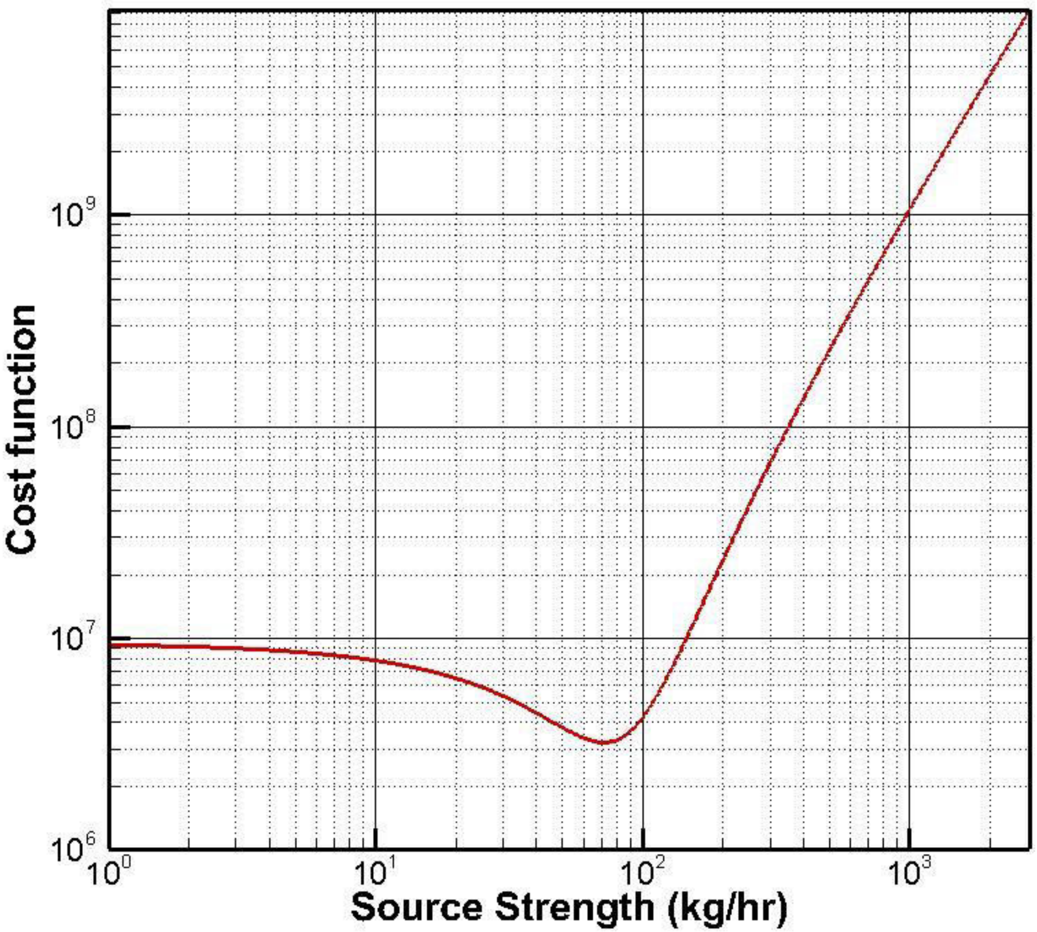


$$\begin{pmatrix} c_1^h \\ c_2^h \\ \vdots \\ c_M^h \end{pmatrix} = \begin{pmatrix} H_{1,1} & H_{1,2} & \cdots & H_{1,N} \\ H_{2,1} & H_{2,2} & \cdots & H_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ H_{M,1} & H_{M,2} & \cdots & H_{M,N} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_N \end{pmatrix}$$



- Solution is the linear combination of release candidates that minimizes the cost function

Estimate the source strength

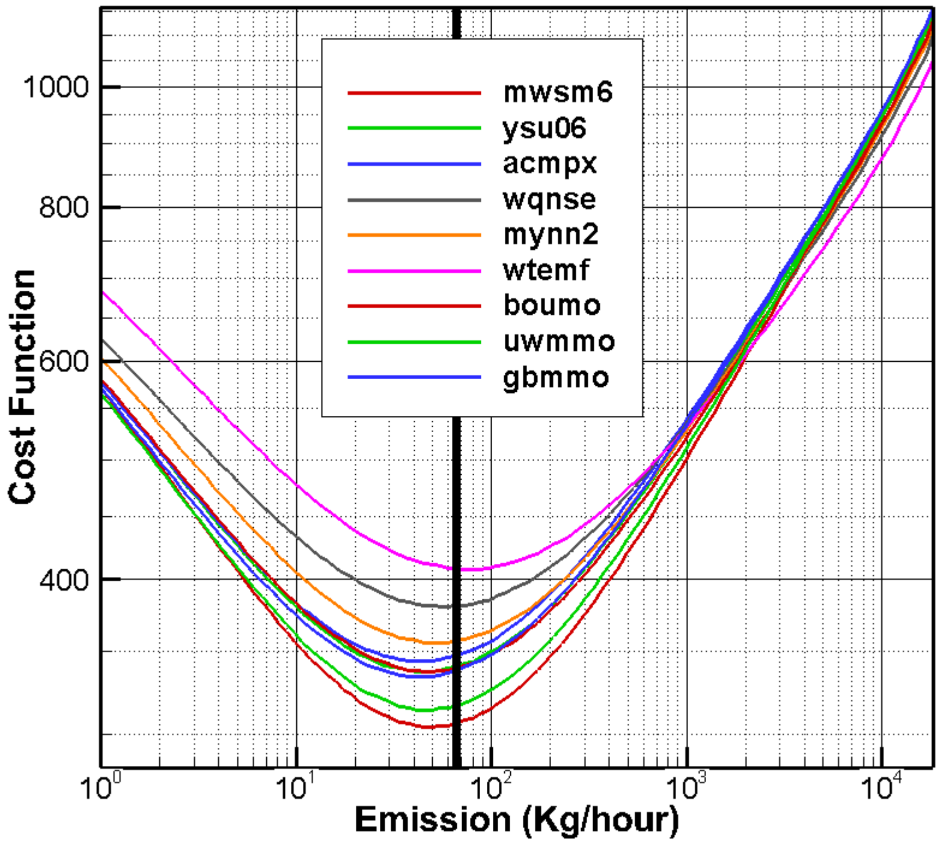


Assumptions:

- Assume release location (Dayton Ohio) is known;
- Exact release starting and ending times (17Z to 20Z on September 25, 1983) are also known.

Release strength corresponding to the minimal cost function gives the source strength estimate as 71 kg/hr, which is 6% larger than the actual release (67 kg/hr).

Estimate the source strength with ensemble



Assumptions:

- Assume release location (Dayton Ohio) is known;
- Exact release starting and ending times (17Z to 20Z on September 25, 1983) are also known.

- An ensemble runs with 9 members with different boundary layer schemes;
- Cost function defined using ln (concentration);
- Estimates: 41 – 73 kg/h

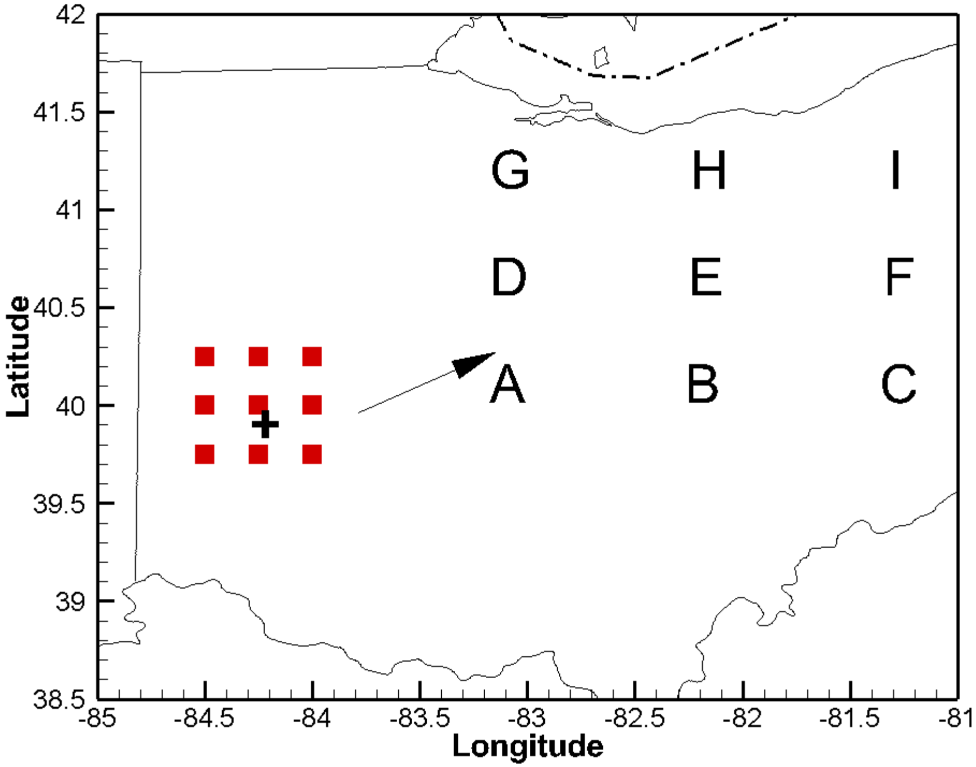
Recover source location

Assumptions:

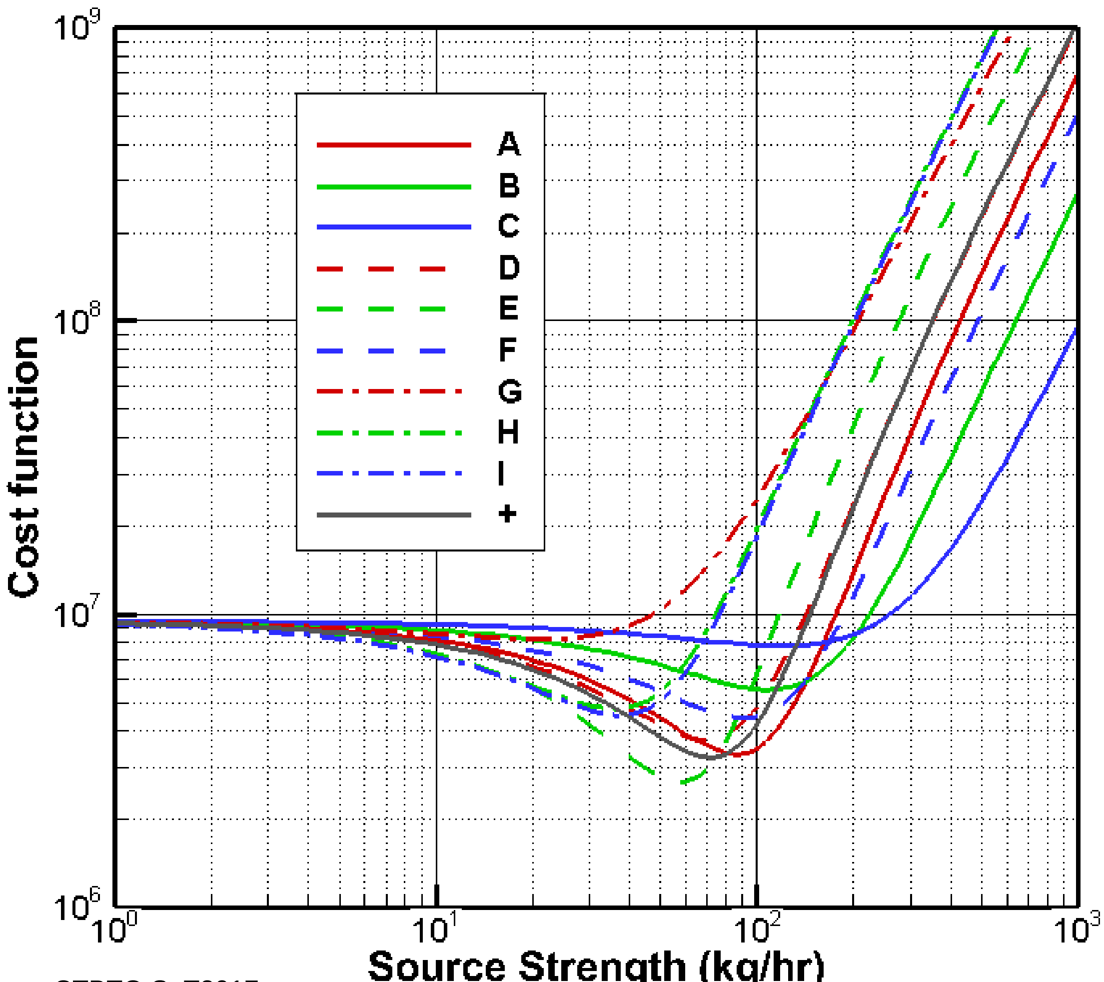
- Exact release time known
- Release strength unknown
- Only one ‘true’ release location
- 9 candidate locations in a 3x3 grid (0.25 degree resolution)

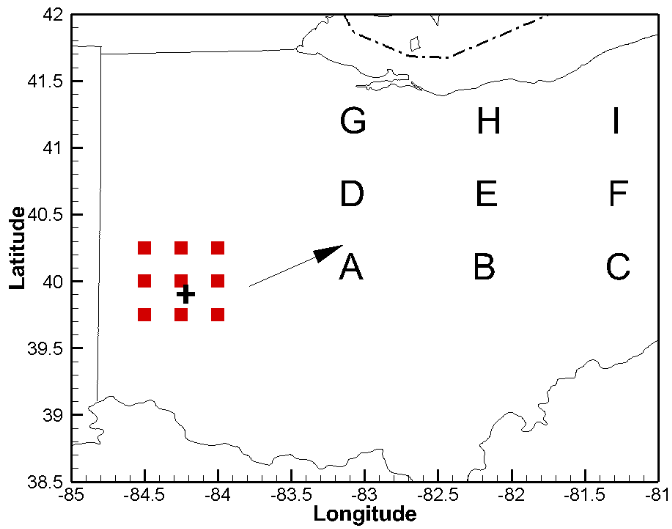
Method:

- Each candidate location is solved independently
- Release location that can generate predictions best matching observations (minimal cost function) as the likely source location.



Identify source location

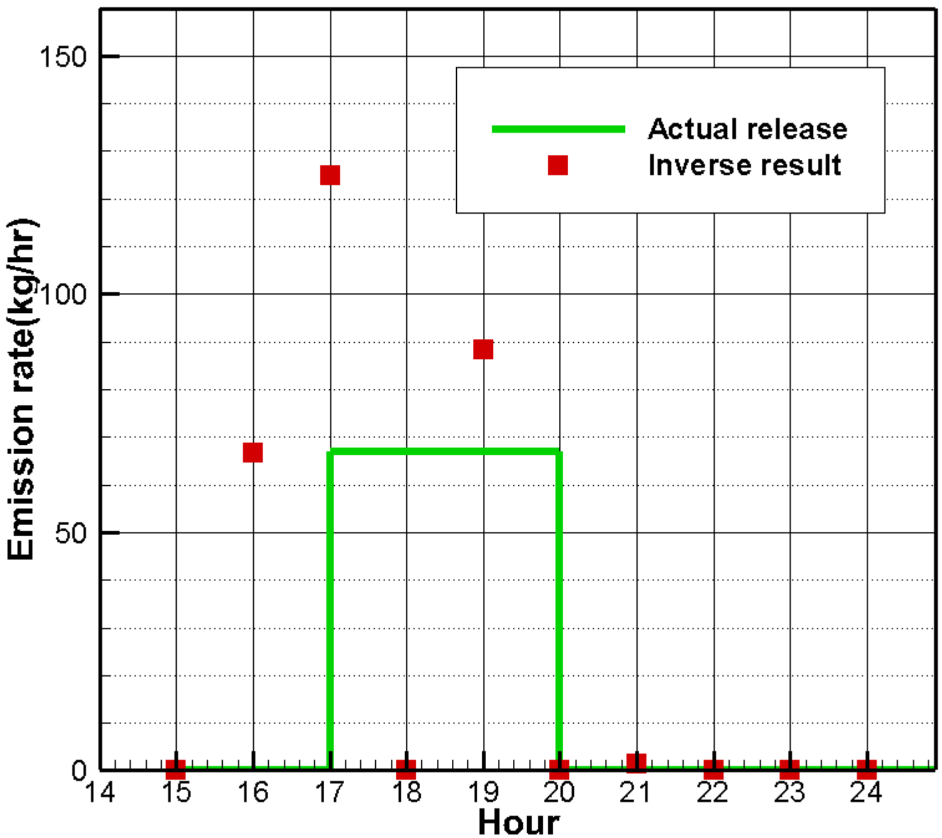




Result:

- Out of the 9 candidate locations, location E (40.00°N, 84.25°W), which is closest to the actual release site (39.90°N, 84.22°W), has the minimal cost function and is identified as the likely source location.
- The source strength is estimated as 58 kg/hr (-13%).
- Location E actually yields a cost function smaller than that from the actual release site.

Recover temporal variations of release



September 25, 1983

Assumptions:

- Assume release location (Dayton Ohio) is known;
- Release could vary hourly;
- Possible release starting at 15Z on September 25, 1983 until last measurement.

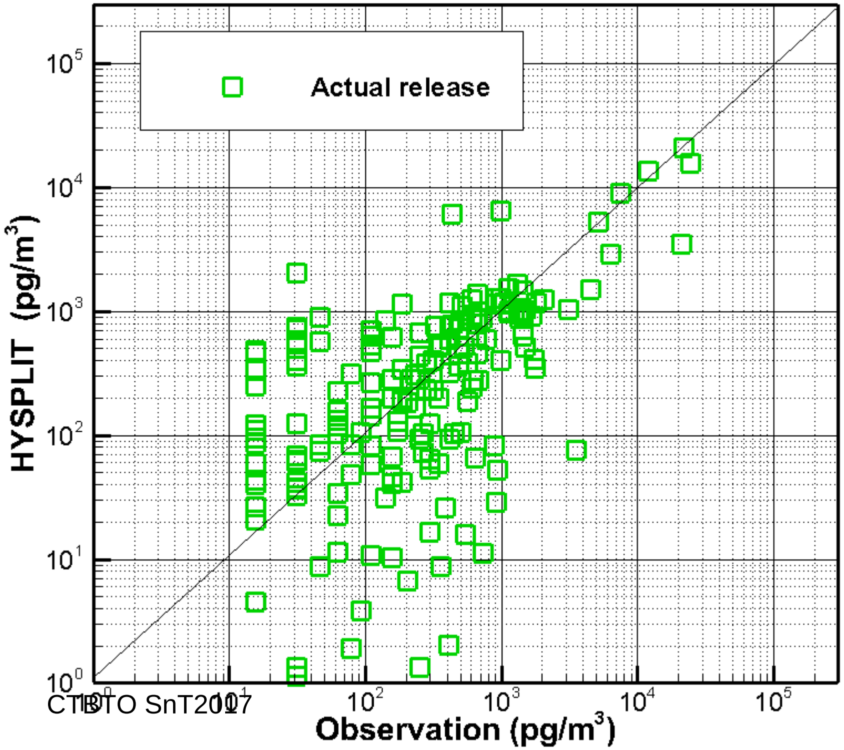
Result:

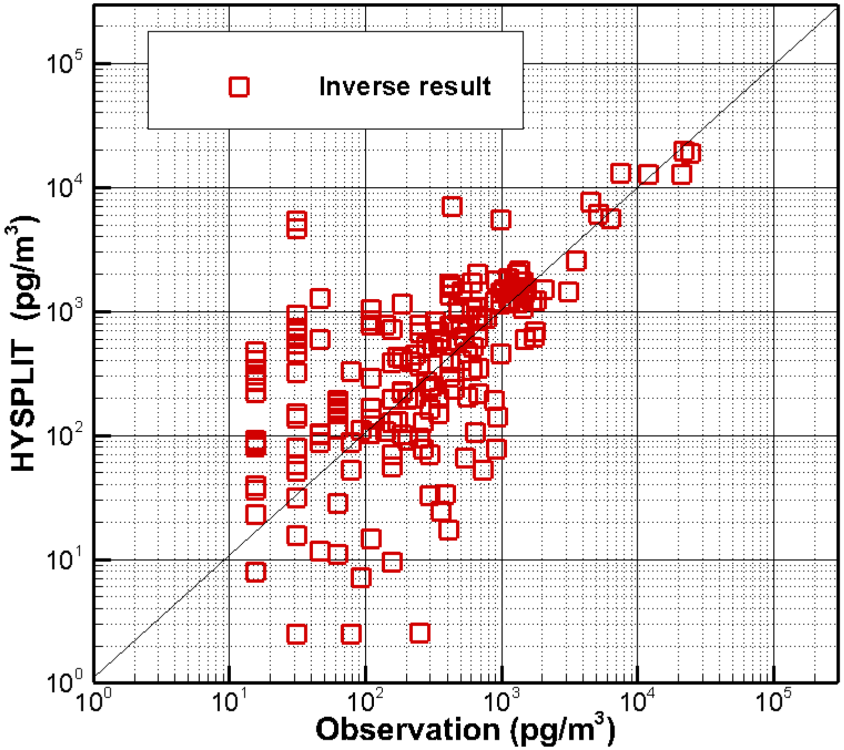
- Releases after 19Z on September 26, 1983 cannot be constrained with available observations;
- Recovered releases after 20Z September 25 are close to 0;
- Temporal variations are different from the actual releases (constant over 3 hours).

Model predictions with two releases

Statistics with two releases. R: correlation coefficient; FB: fractional bias; FMS: Figure of Merit in Space; KSP: Kolmogorov-Smirnov Parameter. Rank: $R^2 + 1-|FB/2| + FMS/100 + (1-KSP/100)$.

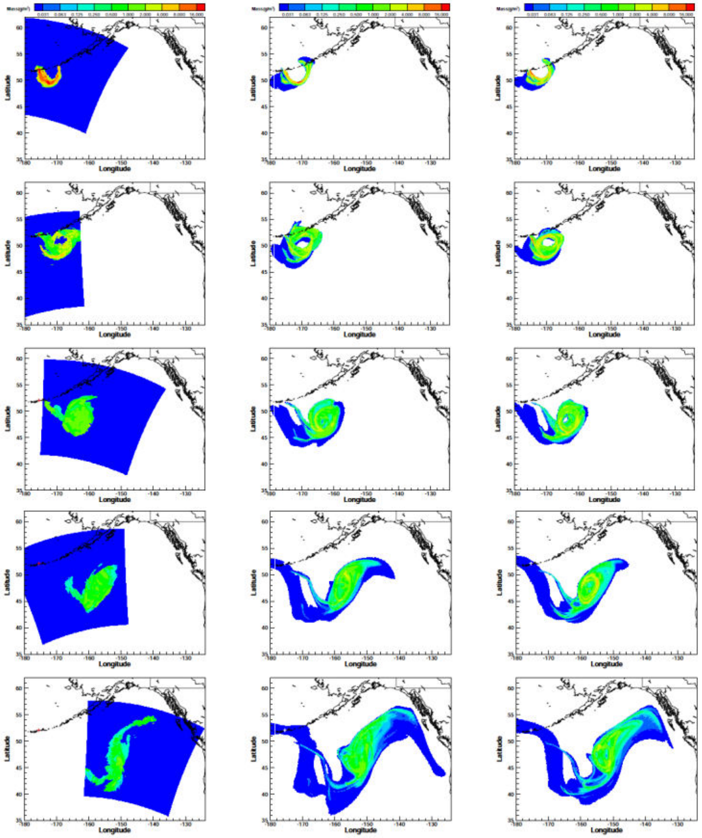
	R	FB	FMS (%)	KSP (%)	Rank
Actual release	0.85	-0.12	73.0	9.5	3.30
Inverse result	0.91	0.19	72.0	10.3	3.36





Use satellite observations to constrain model – *An example with volcanic ash measurements*

- MODIS (Moderate Resolution Imaging Spectroradiometer) satellite retrievals of the 2008 Kasatochi volcanic ash clouds: mass loadings and ash cloud top height;
- Five satellite granules observed at approximately 12 hours apart from each other, with 3788 to 15088 ash cells;
- A total of 290 source terms vary with time (29 hours) at 10 release heights;
- Both GDAS (center) and ECMWF (right) meteorological data are used;
- Model predictions with volcanic ash release estimates show skill when evaluated against the unassimilated satellite observations (last 2 granules).



Improving volcanic ash predictions with the HYSPLIT dispersion model by assimilating MODIS satellite retrievals, Chai, T., Crawford, A., Stunder, B., Pavolonis, M., Draxler, R., and Stein, A., *Atmos. Chem. Phys. Discuss., doi:10.5194/acp-2016-750, in review, 2016.*

Summary

- Emission inversion based on the assimilation of 4D observations using HYSPLIT model, its TCM, and a cost function is applied to CAPTEX experiment ;
- Release strength can be recovered reasonably well if both the release time and location are known;
- Ensemble runs provide a good estimate of uncertainties;
- Release location can be approximately identified with known release time;
- Temporal variations of the release are difficult to recover with available observations;
- More observations may be needed when the number of control variables are increased. Satellite observations provide good constraint to inverse modeling.

Thank you!