Inverse modeling with HYSPLIT Lagrangian dispersion model

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Motivation

The Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model developed at NOAA Air Resources Laboratory has been widely used to study the atmospheric pollutant transport and dispersion in both forward and backward modes. Among those applications, the backward trajectory of a single pollutant particle is often used to identify the potential source locations. An improvement can be made by employing the dispersion module to quantify the source strength by utilizing the concentration information.

HYSPLIT Dispersion Model

HYSPLIT is more than a "trajectory model". HYSPLIT4 allows Lagrangian representations of the transported air masses with 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.

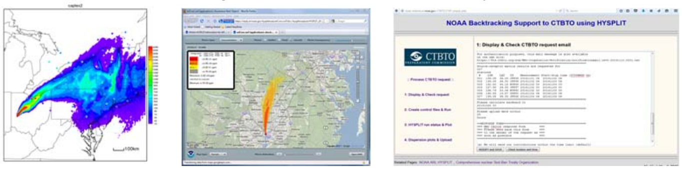


Figure 1. Examples of HYSPLIT dispersion model applications: CAPTEX tracer release experiment, Emergency Response for chemical releases, and CTBTO backtracking support.

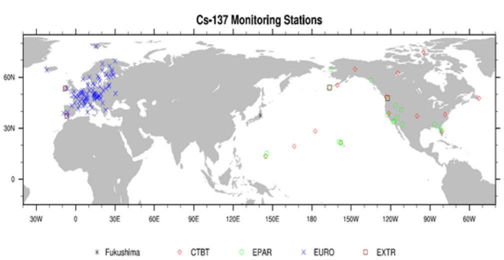
HYSPLIT Inverse Modeling Methodology

In this top-down approach, the unknown emission terms are obtained by searching the emissions that would provide the best model predictions closely matching the observations. For the applications shown here, the emission locations are mostly identified, the unknown emission rates and sometimes the release heights are left to be determined. The emission rates may vary significantly with time. Thus, the unknowns of the inverse problem are the emission rates q_{ikt} at each location i, at different height k and period t. The cost function F is defined as,

$$\mathcal{F} = \frac{1}{2}\sum_{t=1}^{T}\sum_{k=1}^{K}\sum_{i=1}^{I}\frac{(q_{ikt}-q^b_{ikt})^2}{\sigma^2_{ikt}} + \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{M}\frac{(c^h_{nm}-c^o_{nm})^2}{\epsilon^2_{nm}} + \mathcal{F}_{other} \quad (1)$$

where c^o_{nm} is the *m-th* observed concentration or mass loading at time period *n* and c^h_{nm} is the HYSPLIT counterpart. As shown in Equation (1), a background term is included to measure the deviation of the emission estimation from its first guess q^b_{ikt}. The background terms ensures that the problem is well-posed even when there are not enough observations available in certain circumstances. The background error variances σ^2_{ikt} measure the uncertainties of q^b_{ikt}. The observational error variances ϵ^2_{nm} represent the uncertainties from both the model and observations as well as the representative errors. F_{other} refers to the other regularization terms that can be included in the cost function. The optimization problem can be solved using many minimization tools, such as L-BFGS-B package, to get the final optimal emission estimates.

Fukushima Nuclear Accident



Data source	Number of monitoring stations	Count of total samples
CTBT	14	417 (421)
EPAR	19 (20)	35 (39)
EURO	78 (80)	785 (797)
EXTR	4	59 (61)
Total	115 (118)	1296 (1318)

Figure 2. Distribution of Cs-137 monitoring stations and count of 24-hour concentrations.

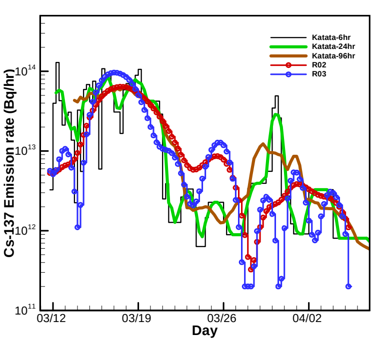


Figure 3. Comparison of HYSPLIT Cs-137 emission estimates and Katata et al. (2015) results. Smoothness parameters are 1.0 and 0.1 for R02 and R03, respectively.

References:

1. 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, *doi:10.1016/j.atmosenv.2015.01.070*, 2015

2. Detailed source term estimation of the atmospheric release for the Fukushima Daiichi Nuclear Power Station accident by coupling simulations of an atmospheric dispersion model with an improved deposition scheme and oceanic dispersion model, Katata, G. and others, *Atmos. Chem. Phys.*, 15, 1029-1070, doi:10.5194/acp-15-1029-2015, 2015.

Volcanic Ash - 2008 Kasatochi Eruption

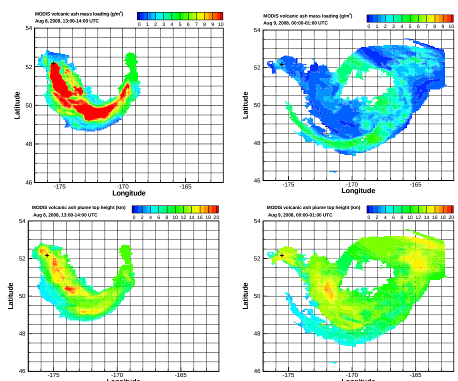


Figure 4. MODIS volcanic ash mass loadings (top row) and ash plume top height (bottom row) of the 2008 Kasatochi eruption in Aleutian Islands (shown with "+"). Left: 13:00-14:00 UTC on Aug 8, 2008; right: 00:00-01:00 UTC on Aug 9, 2008.

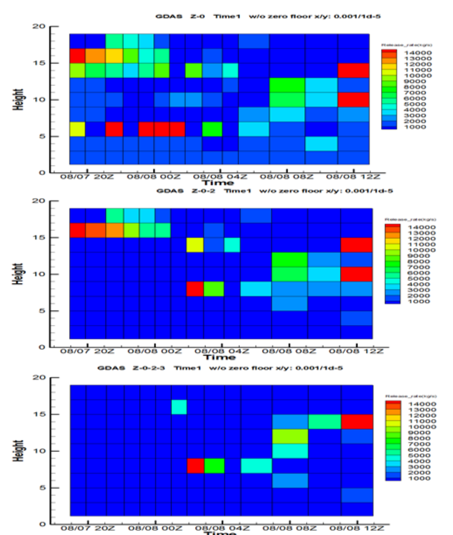


Figure 5. HYSPLIT estimated volcanic ash releases using MODIS ash retrievals at 13:00-14:00 UTC on Aug 8, 2008 with GDAS meteorological data. Top: constrained with non-zero ash; middle: adding clear sky constraints; bottom: adding additional constraints of "no ash above plume height".

Wildfire Smoke

HYSPLIT is used for the operational smoke forecasts in support of the National Air Quality Forecast Capability (NAQFC). While most wild fire locations are well identified by the NOAA NESDIS Hazardous Mapping System (HMS), the current US Forest Service (USFS) BlueSky emission prediction may bring large uncertainties. This research aims to objectively and optimally estimate the wildfire smoke source strengths and their temporal variations based on NOAA NESDIS GOES Aerosol/Smoke products (GASP).

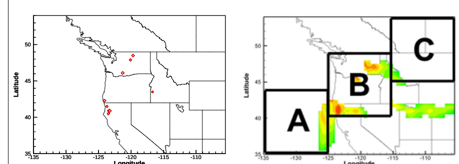


Figure 6. Twin experiments setup. Constant smoke releases at 9 fire locations (shown in the left panel) for two days from 6Z on August 17, 2015, at 1500m or 2000m are simulated by HYSPLIT. Hourly pseudo-observations of satellite mass loadings are generated based on the HYSPLIT results(right panel).

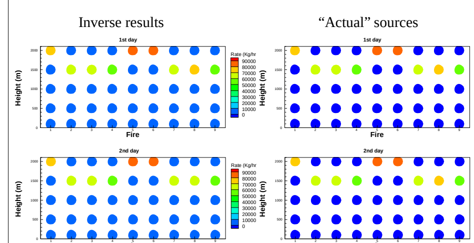


Figure 7. Comparison of the estimated smoke emission rates (left) at the nine locations (fire 1-9 as x-axis) for the two days (upper: 1st day; lower: 2nd day) and the "actual" sources (right) used in the twin experiment.

Table 1. Source term error statistics of the twin experiments

	Source term	MAE (kg/hr)	Normalized MAE	RMSE (kg/hr)	Normalized RMSE
Case 1 : Observations available at all 48 hours	Day 1	534.9	0.77%	841.4	1.21%
	Day 2	1760.5	2.53%	3332.5	4.78%
Case 2 : Observations available at last 24 hours	Day 1	1985.8	2.85%	3310.2	4.75%
	Day 2	1393.0	2.00%	2943.2	4.22%
Case 3: Observations available at last 24 hours; Region A in Fig 7 blocked.	Day 1	606.4	0.87%	1156.3	1.66%
	Day 2	301.2	0.43%	573.4	0.82%
Case 4: Observations available at last 24 hours Region B in Fig 7 blocked.	Day 1	23834.6	34.21%	32157.9	46.16%
	Day 2	66177.5	94.99%	78653.3	112.90%
Case 5: Observations available at last 24 hours Region C in Fig 7 blocked.	Day 1	3974.9	5.71%	8803.3	12.64%
	Day 2	3400.6	4.88%	10663.2	15.31%

Summary, discussion, and future work

1. A HYSPLIT inverse system based on a 4D-Var approach has been built to have a top-down estimation of the emissions by assimilating various observations;
2. The estimated release of the radionuclide caesium-137 using daily average Cs-137 air concentration measurements around the globe from the Fukushima nuclear accident agrees well with the latest estimates by Katata et al. (2015);
3. The HYSPLIT inverse system is then extended for volcanic ash applications, where the release heights are unknown and the HYSPLIT counterparts of the satellite mass loading columns are needed;
4. Preliminary results of the 2008 Kasatochi eruption show the importance of additional constraints which utilize the plume-free regions where the satellites do not observe volcanic ash;
5. The feasibility of applying the method to objectively and optimally estimate wildfire smoke sources based on satellite observations of fire plumes is demonstrated using a set of twin experiments;
6. The twin experiments show that missing satellite observations in key regions could dramatically affect the emission estimations;
7. Finding release locations based on observations and the HYSPLIT model will be studied in the future.

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