CO₂-USA ARL Modeling System Updates

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Introduction

• Goal:

Apply model to estimate carbon emissions and trends in different U.S. cities

• 1st Step:

- Construct an atmospheric modeling system that is scalable and transferable between cities
 - Enhance HYSPLIT with STILT routines
 - Compile urban/suburban scale datasets for testing updated HYSPLIT model
 - Host benchmark scenarios for future testing of model updates and model inter-comparisons

• Benefits of HYSPLIT modeling system updates:

- Enhance HYSPLIT's capabilities
- Host and maintain STILT routines with HYSPLIT code that will continue to be updated with the state of the science
- Provide testing platform to evaluate and examine model similarities and differences to other Lagrangian models / model options. Testing platform can also be used to test inversion techniques to estimate source strength and location.



- Lagrangian emission, transport, dispersion, and deposition. Eulerian complex chemistry.
- Automated method of simultaneously using multiple meteorological grids.
- Multiple parameterizations to estimate the stability from gradients of meteorological variables.
- Multiple options to convert stability into dispersion values (diffusivity profiles, turbulent kinetic energy, velocity variance).
- Modeling the turbulent particle motion directly (3D) or the change in the statistic of the particle distribution (puffs) or a combination of the two.
- Mixed-mode approach: 3D part to puff, 3D part to Eulerian, puff to 3D part, puff to Eulerian.

HYSPLIT meteorological input files

- Pre-processors for many different meteorological models and gridded analysis/reanalysis datasets (WRF, RAMS, MM5, ECMWF, GALWEM, MERRA, ERA interim, ERA5) to convert data to the ARL format, in addition to the archives of existing NOAA models and analysis/reanalysis (NAM, HRRR, GFS, SREF, NARR, GDAS, NCEP/NCAR reanalysis).
- ARL new WRF simulation
 - Resolution: 27 km (216 E->W, 174 S->N, 33 vertical from surface to 100mb)
 - Timeframe: 1980-2016 with plans to continue through 2017 and beyond
 - Domain covers all of CONUS
 - Model configured to obtain optimal transport results; not temperature
 - Some STILT specific optional inputs are available (mass conserving winds available, but no convection variables)
 - Converted to ARL formatted files and is publically available
- Future ARL WRF simulation
 - Resolution: 9 km, nested down from the 27 km domain described above
 - All STILT optional inputs will be available
 - Will be converted to ARL formatted files and made publically available

HYSPLIT Model Evaluation System

Data Archive of Tracer Experiments and Meteorology (DATEM)

• Approach

- Meteorology
 - North American Regional Reanalysis (NARR)
 - WRF runs
- Common statistical evaluation protocols
- Accomplishments
 - Web access to run HYSPLIT for each experiment
 - Standardized model change testing in conjunction with version control



- Cross Appalachian Tracer Experiment (CAPTEX) Dayton, OH, and Sudbury, ONT, Sep., Oct., 1983
- Atlantic Coast Unique Regional Atmospheric Tracer Experiment (ACURATE), Savannah River Plant, SC, Spring 1982 – Summer 1983
- Across North America Tracer Experiment (ANATEX), Glasgow, MT, and St. Cloud, MN, January through March 1987
- Oklahoma Tracer Experiment, Norman, OK, July, 08 1980
- Metropolitan Tracer Experiment (METREX), Washington, DC, January – December 1984
- European Tracer Experiment (ETEX), Rennes, France, October 23, 1994
- Savannah River Plant Experiment , Aiken, SC, Aug. 1975 through Sep. 1977
- Atmospheric Studies in Complex Terrain (ASCOT), California, September 12-25, 1980
- Colorado Springs Tracer Experiment (COSTEX), October 18, 21, 23, 2010
- Sagebrush, Idaho, 2013
- Aliso Canyon well blowout, 2015
- Tracers of opportunity (e.g. SO2 flight data)

STILT

- Built from the HYSPLIT code
- Major STILT features not currently in HYSPLIT:
 - Mass conservation
 - Hanna Lagrangian timescale
 - Convection scheme that utilizes WRF convective fluxes
 - A more complex turbulence module that includes a reflection/transmission scheme for Gaussian turbulence. This preserves well-mixed distributions of particles moving across interfaces between step changes in turbulence parameters.
 - Account for transport errors by incorporating uncertainties in winds into the motion of air parcels

HYSPLIT – STILT Comparison

Average rank results from 8 case studies from HYSPLIT and STILT simulations (Hegarty et al., 2013).

Model	NARR Only	WRF avg PBL=1	WRF avg PBL=0	WRF inst PBL=1	WRF inst PBL=0
HYSPLIT	2.13	2.42	2.34	2.29	2.29
STILT	2.12	2.39	2.26	2.26	2.27

$RANK = R^{2} + (1 - |FB/2|) + FMS/100 + (1 - KS/100)$

- R² = Square of linear correlation coefficient
- FB=Fractional Bias defines a normalized measure of bias
- FMS = Figure of Merit in Space defines a percentage of overlap between measured and predicted areas
- KS = Kolomogorov-Smirnov parameter defines the maximum difference between two cumulative distributions

STILT features being incorporated into HYSPLIT

- Mass Conservation
- Convection scheme
- Hanna Lagrangian timescale
- Complex turbulence module
- Account for transport errors

Allow for updated features to be modular

Testing updated HYSPLIT with STILT features

- Evaluate individual model options over a range of scenarios (field campaigns and computational experiments).
 - What are the differences and similarities between different model options.
 - Document differences in computational time for each model option (speed is of great importance for operational purposes).
 - When is it necessary to use the more complex model option that requires more computational resources?
- Expand the DATEM archive to incorporate field campaign data on the urban / suburban spatial scale.
- Provide meteorological datasets and HYSPLIT simulations for benchmarking to the Lagrangian modeling community. Can be used to test atmospheric dispersion models and inversion techniques.

HYSPLIT simulation of Sagebrush experiment



- Horizontal grid: 27km, 9km, 3km, 1km and 333m
- Vertical coordinate: 33 layers with the 1st mid-layer at around 8m and 20 layers included below 850 hPa.
- Simulation period: 2013/10/07 00UTC 10/08 00UTC

HYSPLIT simulation of Sagebrush experiment



2015 Aliso Canyon blowout

- Large natural gas emissions released from a well blowout of connected to an underground storage facility
- 13 research aircraft flights sampled the plume
- Atmospheric leak rates up to 60 metric tons of methane and 4.5 metric tons of ethane per hour (Conley et al., 2016)





Tracers of Opportunity

- Observations downwind of an isolated source with known emissions rates
- Continuous Emissions Monitoring Systems (CEMS) measures actual emissions from stationary sources.

TEXAQS II



Conclusion

- Add new features (from STILT) into HYSPLIT
- Maintain HYSPLIT's computational efficiency / speed for operational use.
- Provide infrastructure for maintaining STILT features within HYSPLIT
- Test individual model options to seek out model differences / similarities
- Create new DATEM on urban / suburban spatial scales
- Provide meteorological datasets and HYSPLIT benchmark runs for future testing