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# Fossil Fuel Emission Verification Modeling at LLNL

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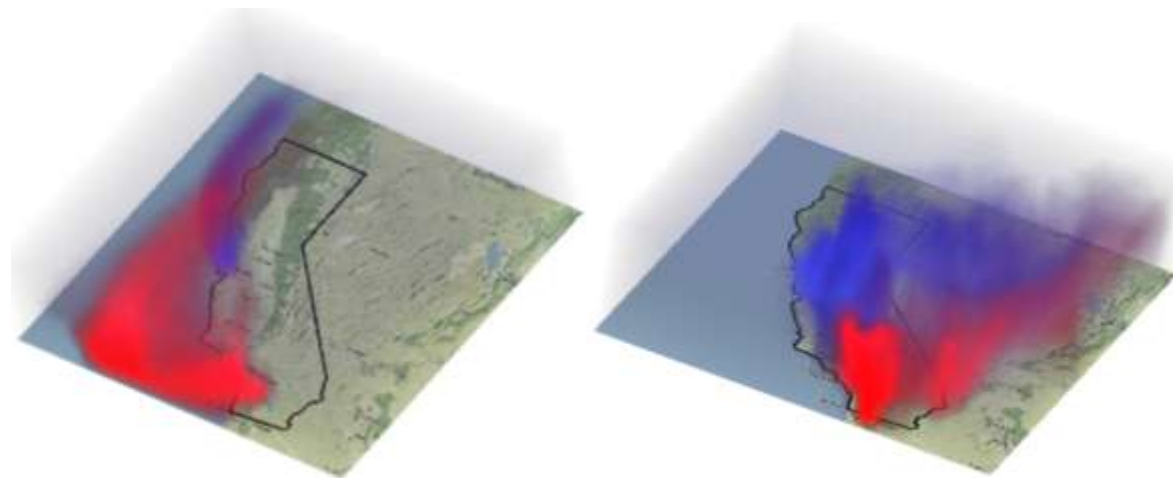
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## Fossil Fuel Emission Verification Modeling at LLNL

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We have an established project at LLNL to develop the tools needed to constrain fossil fuel carbon dioxide emissions using measurements of the carbon-14 isotope in atmospheric samples.

In Figure 1 we show the fossil fuel plumes from Los Angeles and San Francisco for two different weather patterns. Obviously, a measurement made at any given location is going to depend on the weather leading up to the measurement. Thus, in order to determine the GHG emissions from some region using in situ measurements of those GHGs, we use state-of-the-art global and regional atmospheric chemistry-transport codes to simulate the plumes: the LLNL-IMPACT model (Rotman et al., 2004) and the WRF-CHEM community code (<http://www.wrf-model.org/index.php>). Both codes can use observed (aka assimilated) meteorology in order to recreate the actual transport that occurred.



*Figure 1: 3D images of fossil fuel plumes from Los Angeles (red) and San Francisco (blue) for two different weather patterns in January 2006, as generated by the WRF-CHEM model. The intensity of color is proportional to concentration.*

The measured concentration of each tracer at a particular spatio-temporal location is a linear combination of the plumes from each region at that location (for non-reactive species). The challenge is to calculate the emission strengths for each region that fit the observed concentrations. In general this is difficult because there are errors in the measurements and modeling of the plumes. We solve this inversion problem using the strategy illustrated in Figure 2.

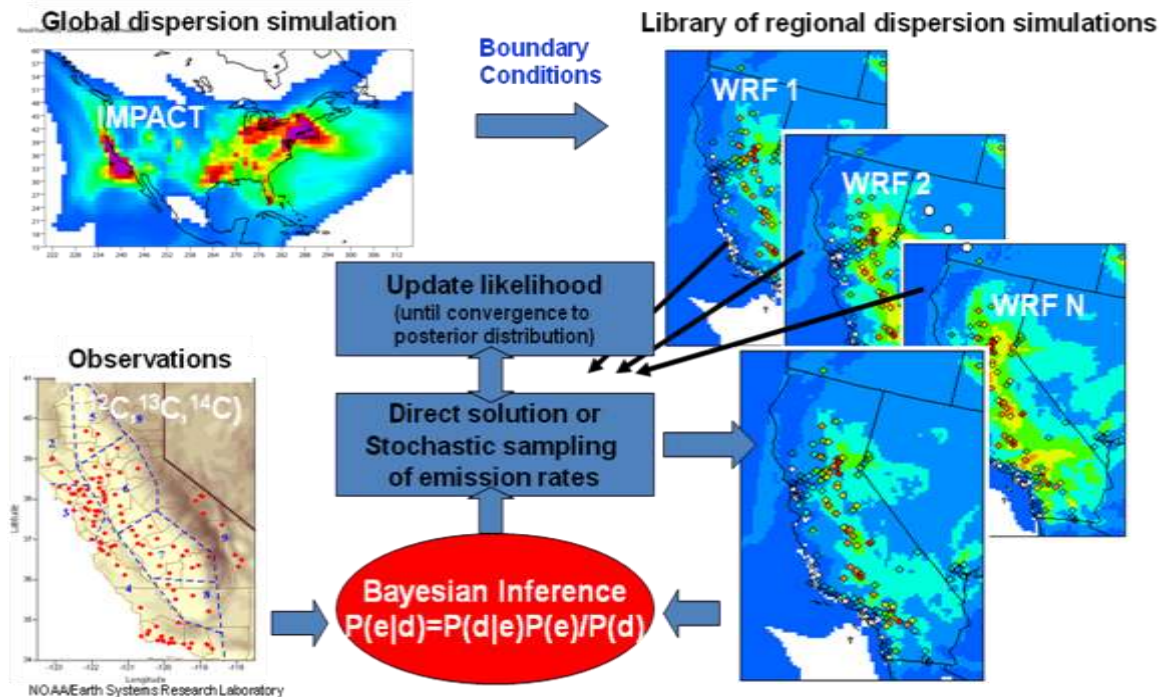


Figure 2: Symbolic representation of our inversion algorithm for retrieving regional emissions.

The Bayesian Inference step combines the *a priori* estimates of the emissions, and their uncertainty, for each region with the results of the observations, and their uncertainty, and an ensemble of model predicted plumes for each region, and their uncertainty. The result is the mathematical best estimate of the emissions and their errors. In the case of non-linearities, or if we are using a statistical sampling technique such as a Markov Chain Monte Carlo technique, then the process is iterated until it converges (ie reaches stationarity).

For the Bayesian inference we can use both a direct inversion capability, which is fast but requires assumptions of linearity and Gaussianity of errors, or one of several statistical sampling techniques, which are computationally slower but do not require either linearity or Gaussianity (Chow, et al., 2008; Delle Monache, et al., 2008).

The emission regions we are using are based on the air-basins defined by the California Air Resources Board (CARB), see Figure 3. The only difference is that we have joined some of the smaller air basins together. The results of a test using 4 days of simulated observations using our ensemble retrieval system are shown in Figure 3 (right). The main source of the variation between the different model configurations arises from the uncertainty in the atmospheric boundary layer parameterization in the WRF model. We are currently developing a capability to constrain the boundary layer height in our carbon-14 work either by weighting the ensemble member results by the accuracy of their boundary layer height (using commercial aircraft observations), or as part of the retrieval process using an ensemble Kalman filter (EnKF) capability.

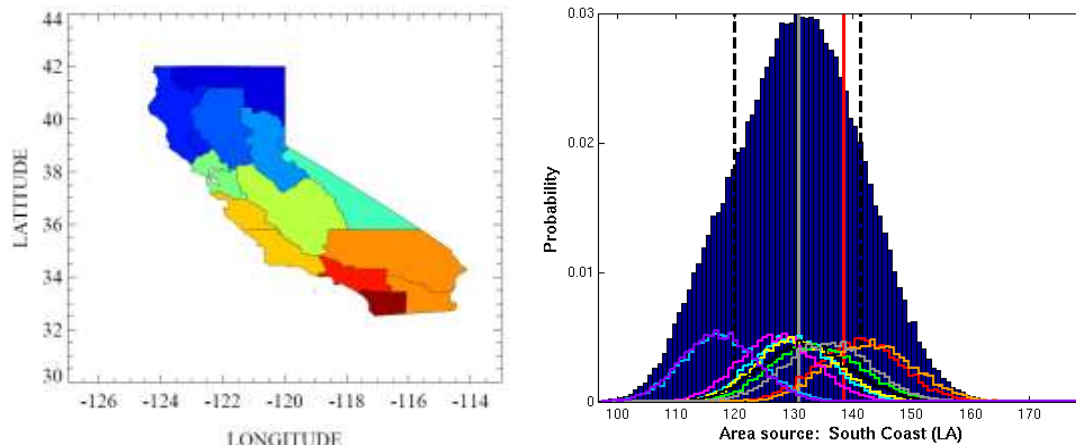


Figure 3: [left] Our independent California emission regions, based on the air-basins defined by the California air resources board. [right] Each colored line shows the retrieved (a posteriori) probability density function (PDF) for fossil fuel CO<sub>2</sub> emissions from a different model configuration (for Los Angeles). The solid blue area shows the combined a posteriori PDF from all the ensemble members. The gray and dashed lines show the median and one standard deviation of the a posteriori distribution, respectively. The red line shows the true value, which lies within the predicted range. These results were based on 4 days of simulated observations

Rotman, D.A.; Atherton, C.S.; Bergmann, D.J.; Cameron-Smith, P.J.; Chuang, C.C.; Connell, P.S.; Dignon, J.E.; Franz, A.; Grant, K.E.; Kinnison, D.E.; Molenkamp, C.R.; Proctor, D.D.; Tannahill, J.R.; "IMPACT, the LLNL 3-D global atmospheric chemical transport model for the combined troposphere and stratosphere: Model description and analysis of ozone and other trace gases", *J. Geophys. Res.*, Vol. 109, No. D4, D04303 10.1029/2002JD003155, 18 February 2004.

Delle Monache, L., Lundquist, J.K., Kosovic, B., Johannesson, G., Dyer, K.M., Aines, R.D., Belles, R.D., Hanley, W.G., Larsen, S.C., Loosmore, G.A., Mirin, A.A., Nitao, J.J., Sugiyama, G.A., Vogt, P.J., 2008: Bayesian inference and Markov Chain Monte Carlo sampling to reconstruct a contaminant source at continental scale. *Journal of Applied Meteorology and Climatology*, 47, 1553-1572.

Chow, F.K., Kosovic, B., and Chan, S.T., 2008: Source inversion for contaminant plume dispersion in urban environments using building resolving simulations. *Journal of Applied Meteorology and Climatology*, 47, 2600-2613.