There is a recent diffusion of data assimilation expertise from numerical weather prediction (NWP) to air quality communities. However, the atmospheric chemistry-transport models (CTM) are still too unstable systems: the perturbations on initial conditions tend to be smoothed out rather than amplified. Therefore, the conclusions from meteorological experiences cannot be applied directly. We perform a comparison study of assimilation algorithms [Wu et al., 2008]. Hopefully this could serve as a base point for the design of assimilation algorithms suitable for one-day ozone forecasts in realistic applications.

Chemistry-Transport Equation for Air Quality Model

\[ \frac{\partial C}{\partial t} + \mathbf{V} \cdot \nabla C = \nabla \cdot \mathbf{D} \nabla C + S \]

Facts
1. Nonlinear due to chemical reaction term
2. High dimension, typically \(10^6\) to \(10^7\);
3. Strong uncertainties mainly due to uncertain parameters [Mallet and Sportisse, 2006]; initial conditions tend to be forgotten.

Assimilation
Estimate the uncertainties for a better prediction from diverse resources, i.e. model simulations, observations and statistics information. Variational vs. sequential algorithms.

1. Model and observations at time step \(k\):
   \[ x_k = H y_k + \gamma_k \quad \text{Obs.} \]
2. Minimization of a cost function \(J(c)\) that deals with:
   \[ J(c) = \frac{1}{2} (c - c_0)^T \mathbf{P}^{-1} (c - c_0) + \frac{1}{2} \mathbf{c}_0^T \mathbf{R}^{-1} \mathbf{c}_0 \]
   where \(c_0 = \mathbf{H}^T \mathbf{P}^{-1} \mathbf{c}_0\).

Implemented Algorithms
1. Optimal interpolation (OI);
2. Ensemble Kalman filter (EnKF);
3. Reduced rank square root Kalman filter (RRSQRT);
4. Four dimensional variational assimilation (4DVar): time interval \(\Delta t = 0...N\).

The parameter sets and perturbation magnitudes are defined in [Wu and Mallet, 2006]. The uncertain parameters sets and their magnitudes are \(\gamma_k\) and \(\gamma_c\), respectively. The two columns of scores for each case show the forecast scores during the assimilation and prediction periods. The bar values are mean scores, and the error bars show the standard deviations over 10 random seed numbers.

Conclusion
It is found that the assimilations significantly improve the ozone forecasts. The comparison results reveal the limitations and the potentials of each assimilation algorithm. In the four-dimensional variational method, it is shown that the model error has to be accounted for to further improve the forecasts. In the sequential methods, the ensemble approach demonstrates great potential for the forecasts during the end of the prediction periods.

References