Handling Model and Calibration Errors In Inversions

Method 1

Define $\mathbf{H} = \mathbf{H}^t + \mathbf{H}^e$

Determine $\mathbf{H}^e$ from multiple runs of different models

Increase measurement error by $\mathbf{H}^e \mathbf{x}^t$

Method 2

As in Method 1, but simply run the filter for an ensemble of different **H** matrices from different models and observation vectors ($\mathbf{y}^0$) with different calibrations chosen to have equal probability (Monte Carlo)

Method 3

Use the state-space evolution equation **($\mathbf{x}(t)=\mathbf{M}(t)\mathbf{x}(t-1) + \mathbf{n}(t)$)** and compute **$\mathbf{Q}=\mathbf{E}(\mathbf{n}\mathbf{n}^T)$** from multiple model **H** values.

UNCERTAINTY ANALYSIS – MODEL AND CALIBRATION ERRORS

(Prinn et al, Science, 292, 1882-1888, 2001)
Kalman Filter took account of random measurement errors (including mismatch errors) only

Other sources of error are:

(1) Assumed [OH] distribution in troposphere:
— from 6 models compute $\overline{[OH]}_j \pm \sigma_{OH}^j$

(2) Assumed destruction frequencies in stratosphere:
— from 3 models compute $\overline{J}_{sj} \pm \sigma_J^j$

(3) Assumed transport rates:
— troposphere/stratosphere exchange time: $\overline{\tau}_{st} \pm \sigma_{st}$
— troposphere meridional exchange times: $\overline{\tau}_{tm} \pm \sigma_{tm}$
— estimate from $CFCl_3$, CF_2Cl_2 observations

(4) Measurement calibration
— from laboratory study and intercalibrations compute calibration factor $\gamma = 1 + \sigma_\gamma$

(5) Assumed industrial emissions
— from industry study compute $\overline{E}_j \pm \sigma_{E_j}$

(6) Chemical rate constants ($OH + CH_3CCl_3$)
— from laboratory studies estimate $k_j \pm \sigma_k^j$

(7) Oceanic loss rates
— from laboratory and field studies estimate $\overline{J}_{ocj} \pm \sigma_{ocj}$

Use Monte-Carlo method:
— 10,000 "equal probability" inversions from random sampling of uncertain variables

Method 1 : Estimate $f = a(t)$ each year to multiply $[OH]_j$ globally or by hemisphere (initialize $a = 1 \pm 1$, $f = 1 \pm 1$)

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See Figure 2. Prinn, R.G., J. Huang, R.F. Weiss, D.M. Cunnold, P.J. Fraser, P.G. Simmonds, A. McCulloch, C. Harth, P. Salameh, S. O'Doherty, R.H.J. Wang, L. Porter, and B.R. Miller, Evidence for substantial variations of atmospheric hydroxyl radicals in the past two decades, Science, 292, 1882-1888, 2001.

Method 2 : Estimate $f = a + b\,P_1(t) + \left(\frac{c}{3}\right) P_2(t)$ to multiply $[OH]_j$ globally or by hemisphere (initialize $a = 1 \pm 1$, $b = 0 \pm 0.01\ \text{year}^{-1}$, $c = 0 \pm 0.01\ \text{year}^{-2}$)

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See Figure 3. Prinn, R.G., J. Huang, R.F. Weiss, D.M. Cunnold, P.J. Fraser, P.G. Simmonds, A. McCulloch, C. Harth, P. Salameh, S. O'Doherty, R.H.J. Wang, L. Porter, and B.R. Miller, Evidence for substantial variations of atmospheric hydroxyl radicals in the past two decades, Science, 292, 1882-1888, 2001.

Table 1

Optimal estimates of global and hemispheric weighted average OH concentrations (conc. 10^3 radical cm^{-3}). OH trends (trend. % $year^{-1}$) and acceleration in OH trends (accel. % $year^{-2}$). The best estimates are considered to be a combination of the content (CON) and annualized content (ACON) methods. The time-averaged total and "process" lifetimes (years) of CH_3CCl_3 (using CON + ACON OH concentrations) are shown. Uncertainties are all 1σ. Quoted errors are the average of the sensitivity and Monte Carlo error estimation methods.

	Global	Northern Hemisphere	Southern Hemisphere
OH conc (CON + ACON)	$9.44^{+1.30}_{-1.31}$	$8.93^{+1.91}_{-2.01}$	$10.05^{+2.06}_{-2.10}$
OH trend (CON + ACON)	$-0.64^{+0.59}_{-0.60}$	$-0.46^{+1.34}_{-1.32}$	$-0.92^{+1.04}_{-1.02}$
OH accel (CON + ACON)	-0.23 ± 0.18	$-0.59^{+0.38}_{-0.41}$	$+0.13 \pm 0.12$
CH_3CCl_3 Lifetime (total)	$4.90^{+0.62}_{-0.49}$	$5.19^{+1.17}_{-0.77}$	$4.58^{+0.94}_{-0.65}$
CH_3CCl_3 Lifetime (trop. OH)	$5.99^{+0.95}_{-0.71}$	$6.32^{+1.81}_{-1.10}$	$5.61^{+1.45}_{-0.93}$
CH_3CCl_3 Lifetime (stratosphere)	$38.87^{+0.34}_{-0.32}$	$41.03^{+0.36}_{-0.32}$	$36.52^{+0.75}_{-0.69}$
CH_3CCl_3 Lifetime (ocean)	$89.01^{+0.27}_{-0.27}$	$99.79^{+0.21}_{-0.23}$	$79.17^{+0.39}_{-0.41}$

Table 2

Optimal estimates of time-averaged (1978-2000) OH concentrations ($10^5 cm^{-3}$) in the lower atmosphere using the average of the content (CON) and annualized content (ACON) methods with separate estimations for the northern and southern hemisphere.

	$90°S - 30°S$	$30°S - 0°$	$0° - 30°N$	$30°N - 90°N$
200-500 hPa	$5.72^{+1.17}_{-1.20}$	$13.23^{+2.71}_{-2.76}$	$11.32^{+2.42}_{-2.55}$	$5.20^{+1.11}_{-1.17}$
500-1000 hPa	$5.47^{+1.12}_{-1.14}$	$15.32^{+3.14}_{-3.20}$	$12.87^{+2.75}_{-2.90}$	$5.79^{+1.24}_{-1.30}$

Residuals For Variable OH Versus Constant OH

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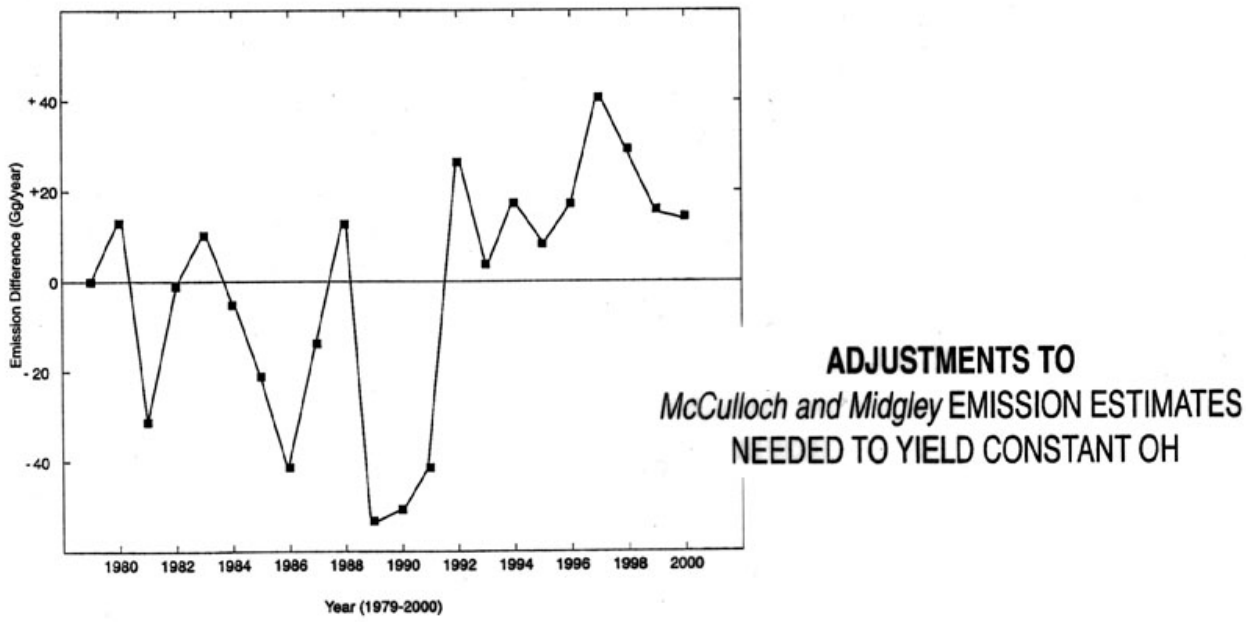
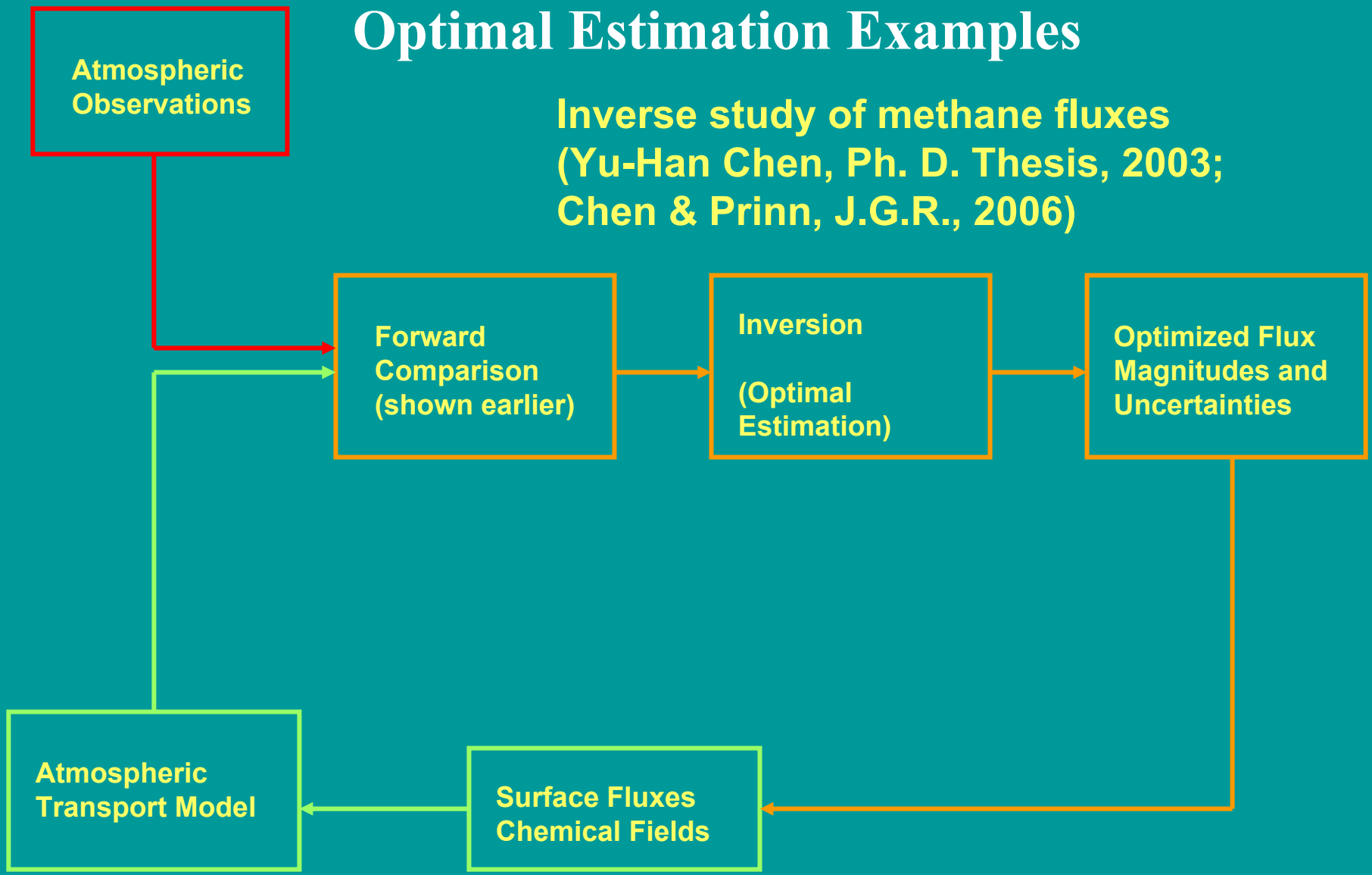
See Figure 4. Prinn, R.G., J. Huang, R.F. Weiss, D.M. Cunnold, P.J. Fraser, P.G. Simmonds, A. McCulloch, C. Harth, P. Salameh, S. O'Doherty, R.H.J. Wang, L. Porter, and B.R. Miller, Evidence for substantial variations of atmospheric hydroxyl radicals in the past two decades, Science, 292, 1882-1888, 2001.



Optimal Estimation Examples



METHANE INVERSE STUDIES USING MATCH

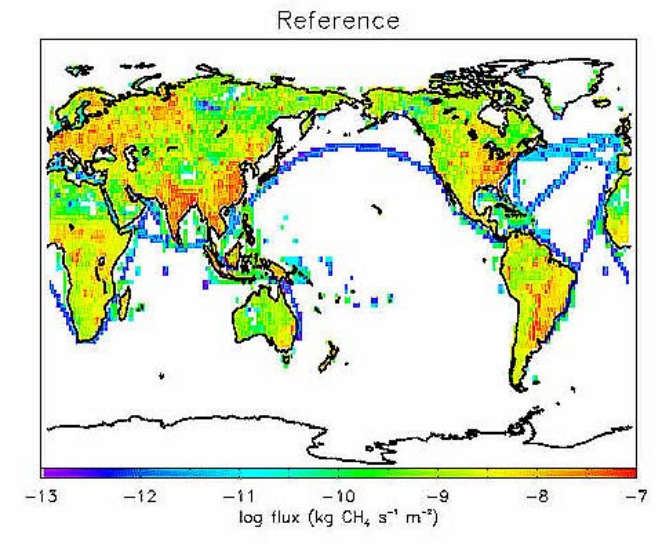
- High-Frequency (13:AGAGE,CMDL,etc) and Flask (41 comprehensive & 32 more intermittent:CMDL,CSIRO,etc.) monthly mean observations between 1996-2001

- Interannually varying transport (NCEP) used in 3D MATCH model to create the CH_4 response of each site to monthly pulses from individual regional processes (sensitivity matrix)

- Kalman Filter used to solve for:
  - 7 Seasonally-varying processes as monthly varying fluxes
  - 3 Pseudo-steady processes as constant fluxes

  using annually repeating time/space varying model OH tuned to AGAGE CH_3CCl_3 observations

Emissions from seven seasonally varying (3 wetland, 3 burning, rice) & two steady sources (animals & waste, coal & gas) to be optimally estimated as amendments to the (a priori) reference



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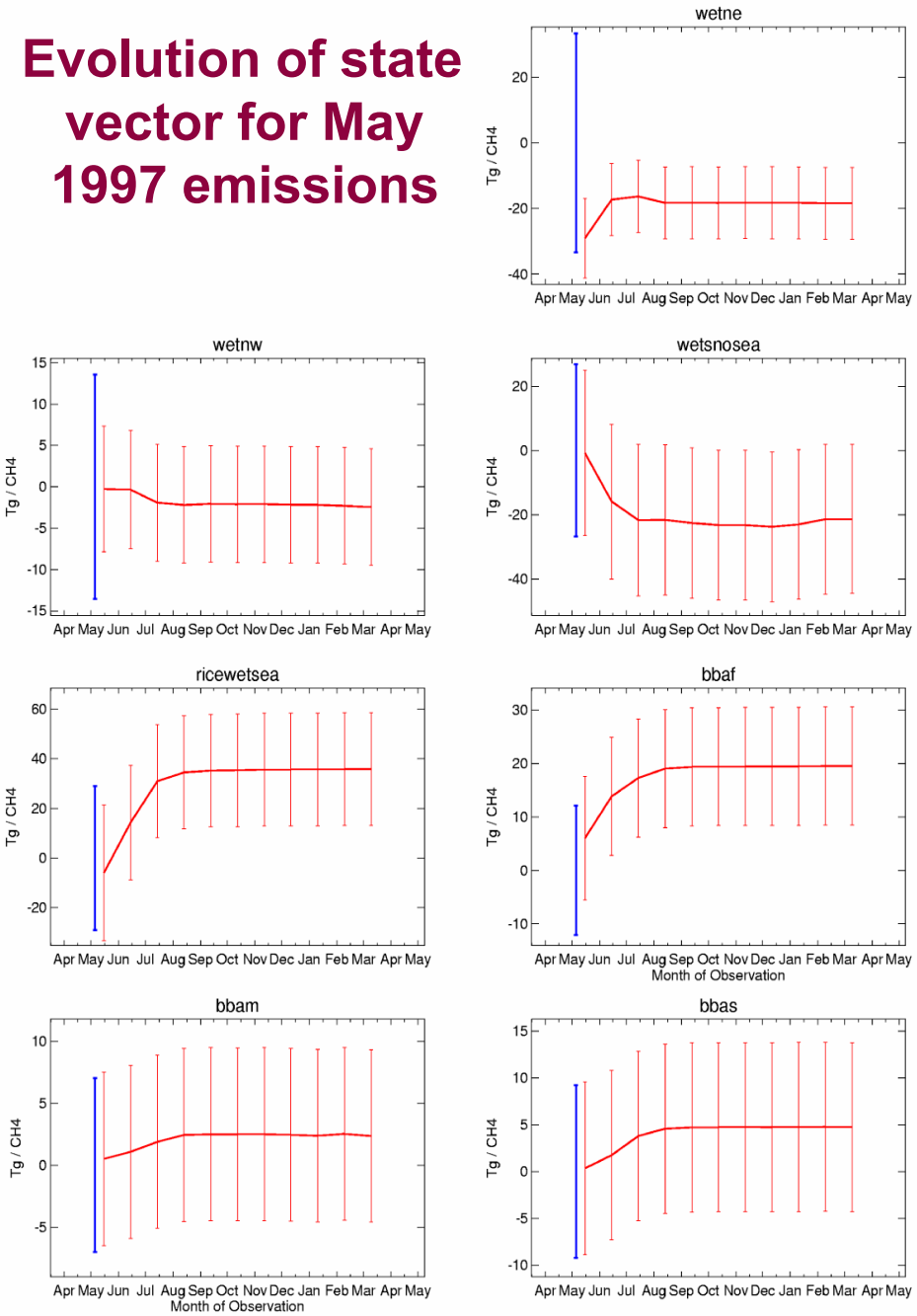
See Figure 2. Chen, Y.-H. and R.G. Prinn, Estimation of atmospheric methane emissions between 1996-2001 using a 3D global chemical transport model, Journal of Geophysical Research, 111, D10307, doi:10.1029/2005JD006058, 2006.

Evolution of state vector for May 1997 emissions



The inverse method uses the transition matrix (M) to remove each monthly flux after it has been estimated for 12 months in the state vector, and adds the latest monthly flux to be estimated