We now use the criterion of optimality to determine K_k. Since we will assume we know $p(y^o)$ and $p(x^t)$, we will choose a value for K_k which minimizes the cost function J (equation 12) for the minimum variance Bayes estimate. Specifically

$$\begin{aligned} J_k &= E[(\nu_k^a)^T \nu_k^a] \\ &= \text{trace}[P_k^a] \end{aligned} \tag{19}$$

Evaluating $\partial J_k / \partial K_k = 0$ and solving for the so-called "Kalman Gain" matrix K_k we have

$$K_k = P_k^f H_k^T [H_k P_k^f H_k^T + R_k]^{-1} \tag{20}$$

Substituting (20) into (18) then yields

$$P_k^a = [I - K_k H_k] P_k^f \tag{21}$$

Finally, using the state space equation (7)

$$x(t) = M(t, t_o) x(t_o) + \eta(t, t_o)$$

we then obtain the estimates of x_k^f needed in (15) and P_k^f needed in (21)

$$x_k^f = M_{k-1} x_{k-1}^a \tag{22}$$

$$P_k^f = M_{k-1} P_{k-1}^a M_{k-1}^T + Q_{k-1} \tag{23}$$

where $Q_{k-1} = E[\eta_{k-1} \eta_{k-1}^T]$, and x_{k-1}^a and P_{k-1}^a are the optimal outputs from the previous iteration of the filter. From our earlier discussion (Section 3), Q could represent random forcing in the system model due to transport model errors.

To use the filter we must provide initial (a priori) estimates for x and P. Then from any prior output estimates (x_{k-1}^a, P_{k-1}^a), we use measurement k information (y_k^o, R_k) and model information (H_k, Q_k) together with equations (22), (23), (20), (15), and (21) to provide outputs x_k^a and P_k^a for inputs to the next step. The filter equations are summarized in Table 1.

Some intuitive concepts regarding the DKF are useful in understanding its operation. First, from equation (20), the gain matrix $K_k \to H_k^{-1}$ (its "maximum" value) as the measurement error covariance (noise) matrix $R_k \to 0$, and $K_k \to P_k^f H_k^T R_k^{-1}$ (its "minimum" value) as $R_k \to \infty$. Since the update in the state vector $x_k^a - x_k^f$ varies linearly with K_k, it is clear that measurements noisy enough so that R_k much exceeds $H_k P_k^f H_k^T$, will contribute much less to improvement of the state vector estimation.

In this respect we can usefully consider $H_k P_k^f H_k^T$ as the error covariance matrix for the measurement estimates y_k. This emphasizes the importance of the weighting of the data inherent in R_k and the distortions created if erroneous R_k are used. Note that R_k can include model error, mismatch error, and instrumental error as noted earlier.

Second, using (21), and recognizing that the maximum value of $K_k H_k = I$, we see $P_k^a \leq P_k^f$ with equality occurring for infinitely noisy measurements. Hence, the error covariance matrix P_k (whose diagonal elements are the variances of the state vector element estimates) decreases by amounts sensitively dependent on the measurement errors.

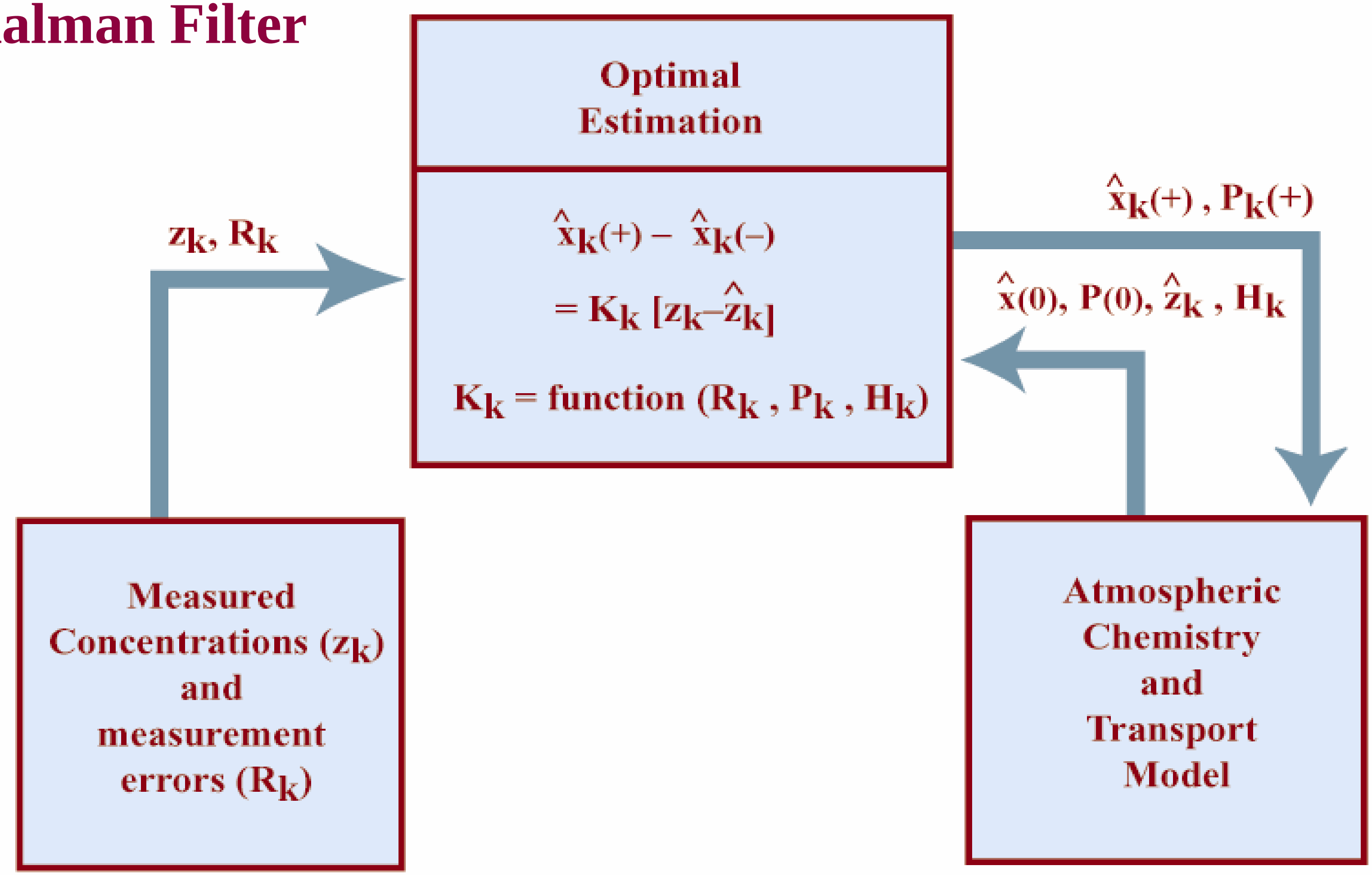
Third, we note from (23), that random forcings η in the system (state-space) model [equation (7)], which are represented here by Q, will increase the extrapolated error covariance matrix P_k^f by amounts depending on the relative values of Q_{k-1} and the extrapolation matrix $M_{k-1} P_{k-1}^a M_{k-1}^T$ in the absence of system (state-space) model noise. The inclusion of Q lessens the influence (or memory) of previous iterations in the filter operation. In the extreme, sufficiently large values of Q will prevent the capability of even non-noisy measurements to decrease P_k and hence increase the confidence in the state vector estimate. In other words excellent (non-noisy) measurements are of little use if the system (state-space) model is very noisy (e.g., through random variations η introduced by random transport errors).

Table 1: Kalman Filter Equations*

Definition	**Equation**
Measurement equation (model)	$y_k^o = H_k x_k^t + \varepsilon_k; \quad y_k = H_k x_k^f$
System (state) equation (model)	$x_k = M_{k-1} x_{k-1} + \eta_{k-1}$
State update	$x_k^a - x_k^f = K_k (y_k^o - y_k)$
Error Update	$P_k^a = (1 - K_k H_k) P_k^f$
Kalman gain update	$K_k = P_k^f H_k^T (H_k P_k^f H_k^T + R_k)^{-1}$
State time extrapolation	$x_k^f = M_{k-1} x_{k-1}^a$
Error time extrapolation	$P_k^f = M_{k-1} P_{k-1}^a M_{k-1}^T + Q_{k-1}$
System random forcing covariance	$Q_k = E(\eta_k \eta_k^T)$
Measurement error covariance	$R_k = E(\varepsilon_k \varepsilon_k{}^T)$
Estimation error covariance	$P_k = E(\nu_k \nu_k{}^T)$
Input measurement matrix	$= H_k = \partial y_k / \partial x_k$
Input system random forcing covariance	$= Q_k$
Input state extrapolation	$= M_k$
Input measurement	y_k^o
Input measurement error covariance	$= R_k$
Filter iteration	$- - - \rightarrow (k-1)^f, \rightarrow$ estimate $\rightarrow (k-1)^a, \rightarrow$ extrapolate $\rightarrow (k)^f, \rightarrow - - -$

*A superscript a or superscript f denotes respectively the value before (f) or after (a) an update of an estimate using measurements, and k denotes the measurement number. In general, errors are assumed random with zero mean and measurement and estimation errors are uncorrelated.

Kalman Filter



Notes on slide notation:

(+) = a, (-) = f, z = y, (^) = model

EXAMPLE

ESTIMATION OF LIFETIME OF CH_3CCl_3 (AND HENCE OH)

Principal Sink is $CH_3CCl_3 + OH \xrightarrow{k} CH_2CCl_3 + H_2O$

Image removed due to copyright considerations.

See: Plate 1. Prinn, R.G., Measurement equation for trace chemicals in fluids and solution of its inverse, in *Inverse Methods in Global Biogeochemical Cycles*, ed. P. Kasibhatla et al., *Geophysical Monographs*, 114, American Geophysical Union, pgs. 3-18, 2000.

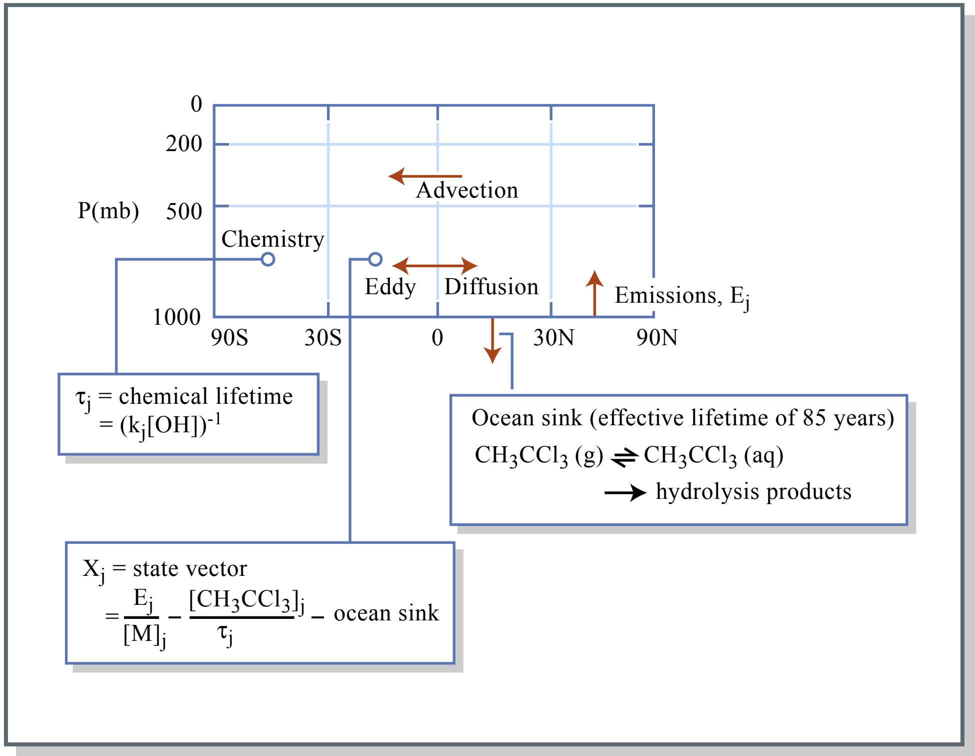


Figure by MIT OCW.

Image removed due to copyright considerations.

See: Figure 3. Prinn, R.G., Measurement equation for trace chemicals in fluids and solution of its inverse, in *Inverse Methods in Global Biogeochemical Cycles*, ed. P. Kasibhatla et al., *Geophysical Monographs*, 114, American Geophysical Union, pgs. 3-18, 2000.

Method: (12)

(1) Multiply reference set of $\frac{1}{\tau_j}$ by unknown parameter α

(2) Multiply mole fractions by unknown calibration factor γ

(3) Estimate state vector $x = \begin{pmatrix} \alpha \\ \gamma \end{pmatrix}$

(4) Compute global average τ from α

Image removed due to copyright considerations.

See: Figure 4. Prinn, R.G., Measurement equation for trace chemicals in fluids and solution of its inverse, in *Inverse Methods in Global Biogeochemical Cycles*, ed. P. Kasibhatla et al., *Geophysical Monographs*, 114, American Geophysical Union, pgs. 3-18, 2000.

Smoother Combines The Forward And Backwards Filters

Notes: (1) $P_k(+) \leq P_k(-)$ so errors decrease with more data

(2) R_k smaller in later years so convergence more rapid running method backwards

(3) Errors include measurement errors but do not include model or emissions errors

(4) Uncertainties meander outside prior uncertainty ranges suggesting errors like (3) important or τ is time varying

Checking your answer:

Compare y^o_k versus y_k

Image removed due to copyright considerations.

See: Figure 5. Prinn, R.G., Measurement equation for trace chemicals in fluids and solution of its inverse, in *Inverse Methods in Global Biogeochemical Cycles*, ed. P. Kasibhatla et al., *Geophysical Monographs*, 114, American Geophysical Union, pgs. 3-18, 2000.