Parameter estimation strategies — transport properties of water in thin film polymers

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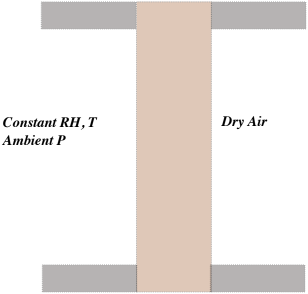
WVTR Experiment



- Measurements taken with MOCON Permatran
- Output of experimental measurement is time trace of water vapor transport rate

Fickian Diffusion Model

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} D \frac{\partial C}{\partial x}$$

- Dirichlet boundary conditions:
  - $C = k_D a$ at $x = 0$
  - $C = 0$ at $x = L$
  - a is activity; $a = (RH) \left. \frac{P_{\mathrm{sat}}}{P_{\mathrm{a}}} \right|_{T_{\mathrm{amb}}}$
- Closed form solution

$$\mathrm{WVTR} = \frac{DKa}{L} \sum_{n=0}^{\infty} 2(-1)^n e^{-Dn^2\pi^2(t-t_0)/l^2} \qquad (1)$$

Global fitting

We also have the functional form:

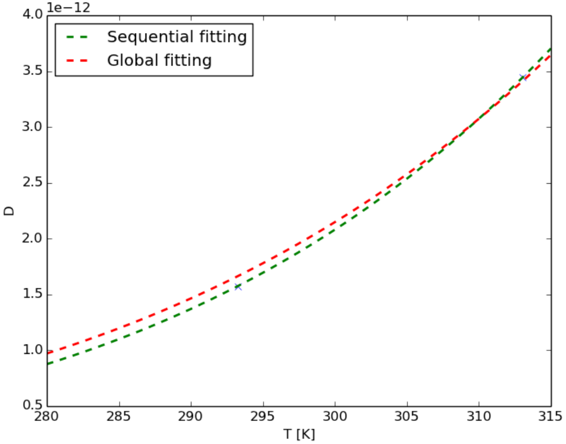
$$D = D_0 e^{D_1/T}$$

$$K = K_0 e^{K_1/T}$$

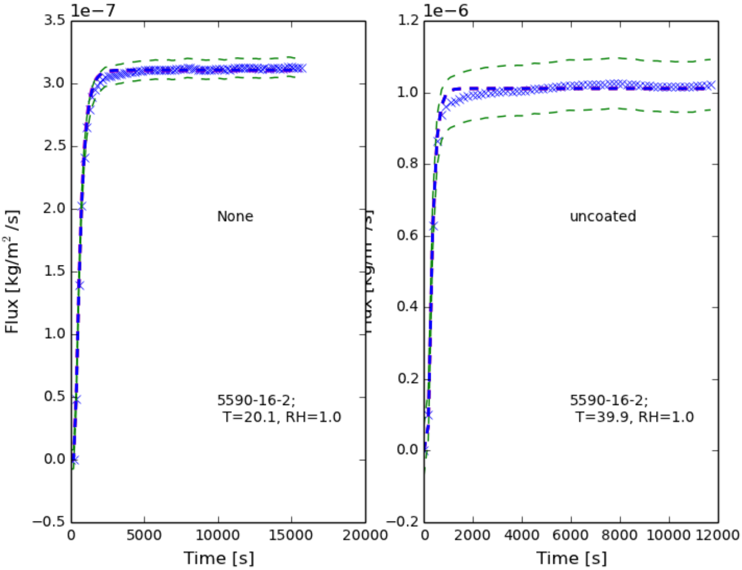
...and experimental data a several different temperatures.

Traditional (MLE?) fitting

- Fit functional form by LS to estimate D, K for each experiment (sequential, then combine into global)
- Fit these directly to global functional form

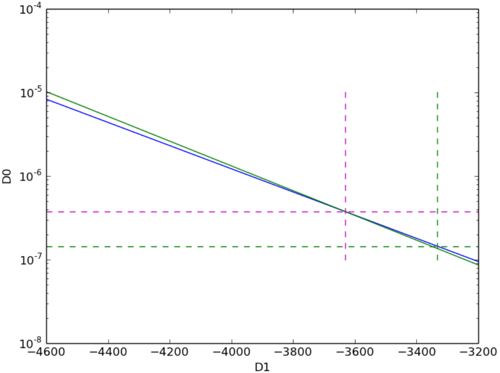


Traditional (MLE?) fitting



Incremental information

- Getting the global fit is slow, even for these 4 experiments (why?)
- At some level this is daft, the search space should be confined to a single $D0$ vs $D1$ line based on the first experiment, but the global fit searches the entire space - which, I think, is why the sequential fit is so much faster
- That being said, running downhill along the line only makes sense if there is a unique solution - i.e., all of these lines intersect at a single point (and they don't)



MCMC Setup

$$L = \frac{1}{2} \sum \frac{(M_i - S_i)^2}{(\sigma_m)_i^2}$$

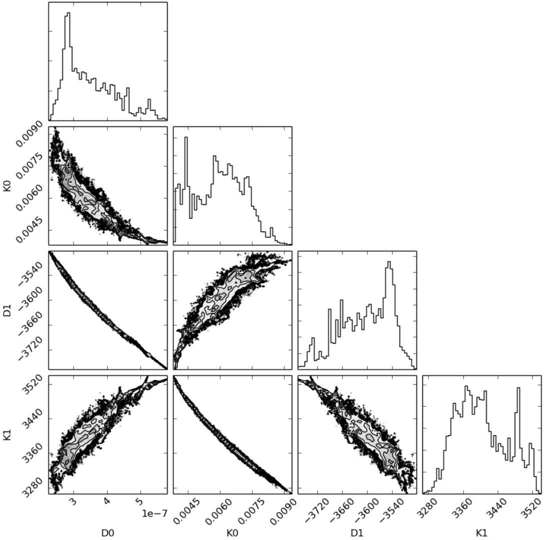
A Gaussian prior would be:

$$P = \frac{1}{2} \left[(\text{prior mean}) - \text{prior}\right]^2 \frac{1}{\sigma_{\text{prior}}^2}$$

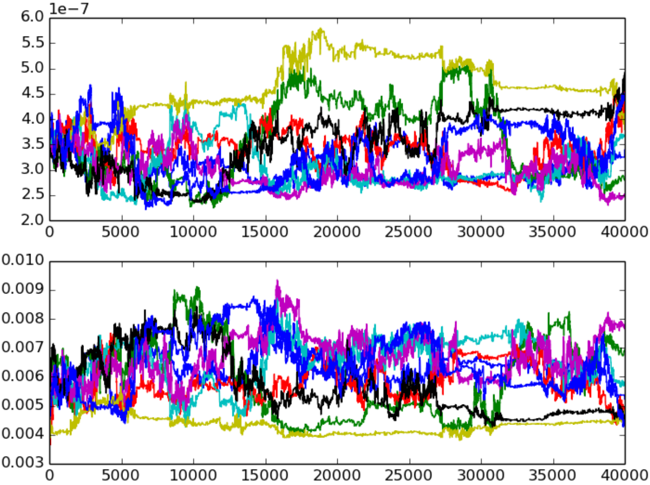
Whereas a uniform prior can be used for an uniformative prior. This was used in the sampler based optimization.
The lnlikelyhood is:

$$-(F_a + F_b) = -(P + L)$$

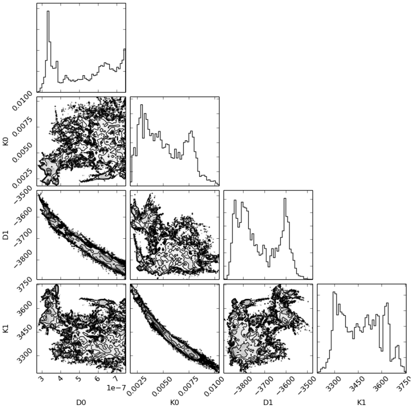
Triangle plot form sampling first two experiments together

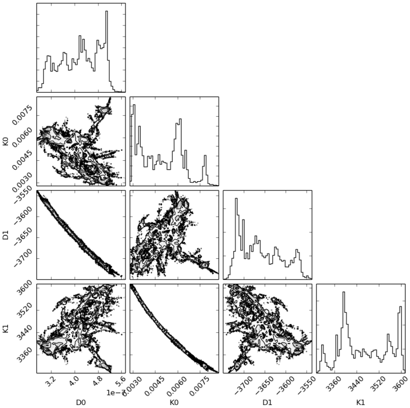


Sample chanins for sampling first two experiments together

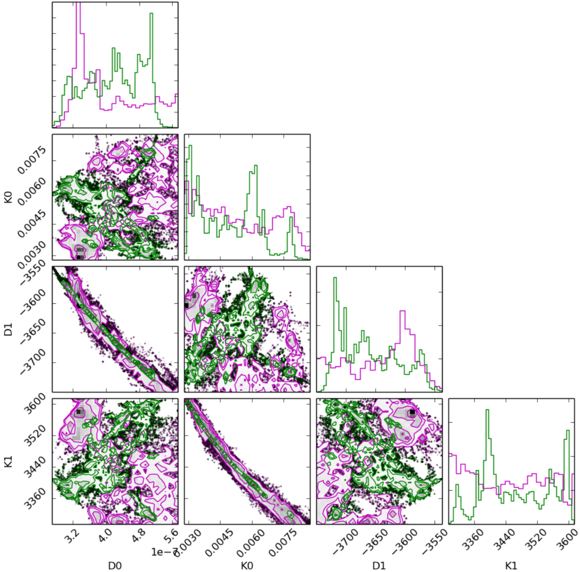


Separate triangle plots from sampling for the 2 experiments independently

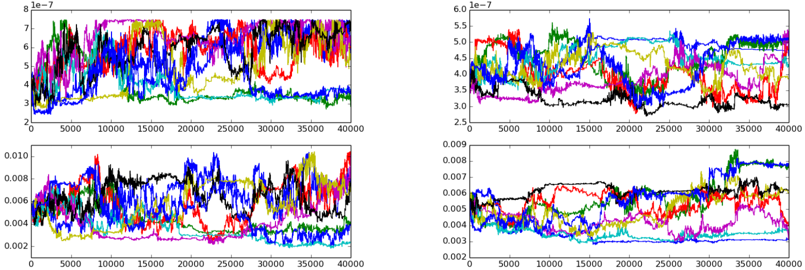




Overlayed triangle plots from sampling for the 2 experiments independently

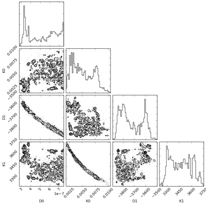


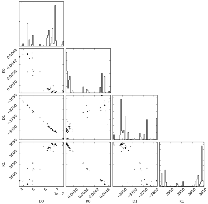
Sample chains for sampling the 2 experiments independently



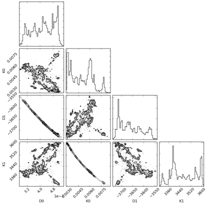
Rescaling

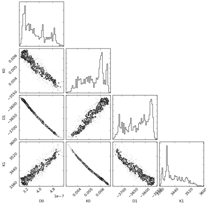
- Rescaling exp 0 by exp 1 ($2400 \to 14$)



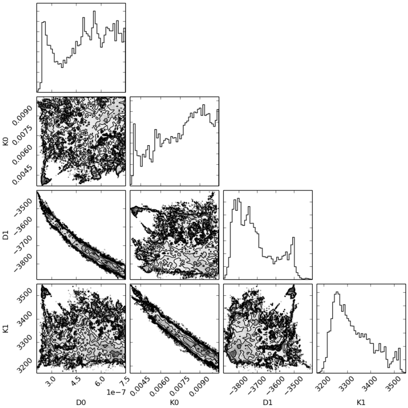


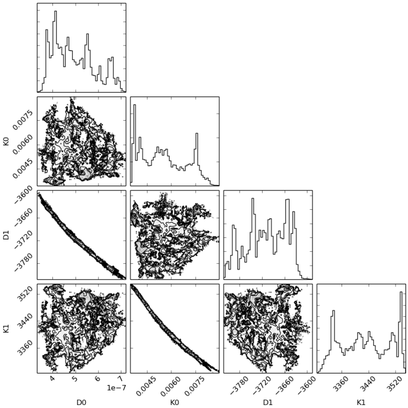
- Rescaling exp 1 by exp 0 ($2400 \to 945$)



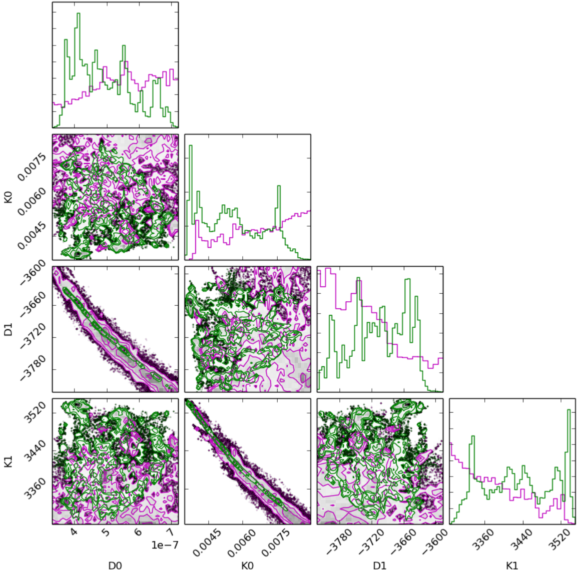


Separate triangle plots from sampling for the 2 experiments using posterior from first as prior for second

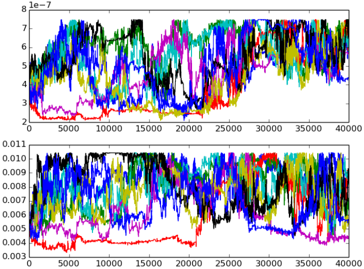


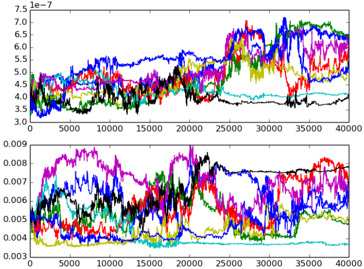


Overlayed triangle plots from sampling for the 2 experiments using posterior from first as prior for second



Sample chains for sampling the 2 experiments using posterior form first as prior for second





Implicit sampling

- Use solution from '2-step' fitting as starting location
- Inverse Hessian from covariance of samples from combined problem (global samples)