Probabilistic Collocation Method (PCM) for modeling response of GEOS-Chem simulations to model parameter uncertainties

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GEOS-Chem Simulation of POPs

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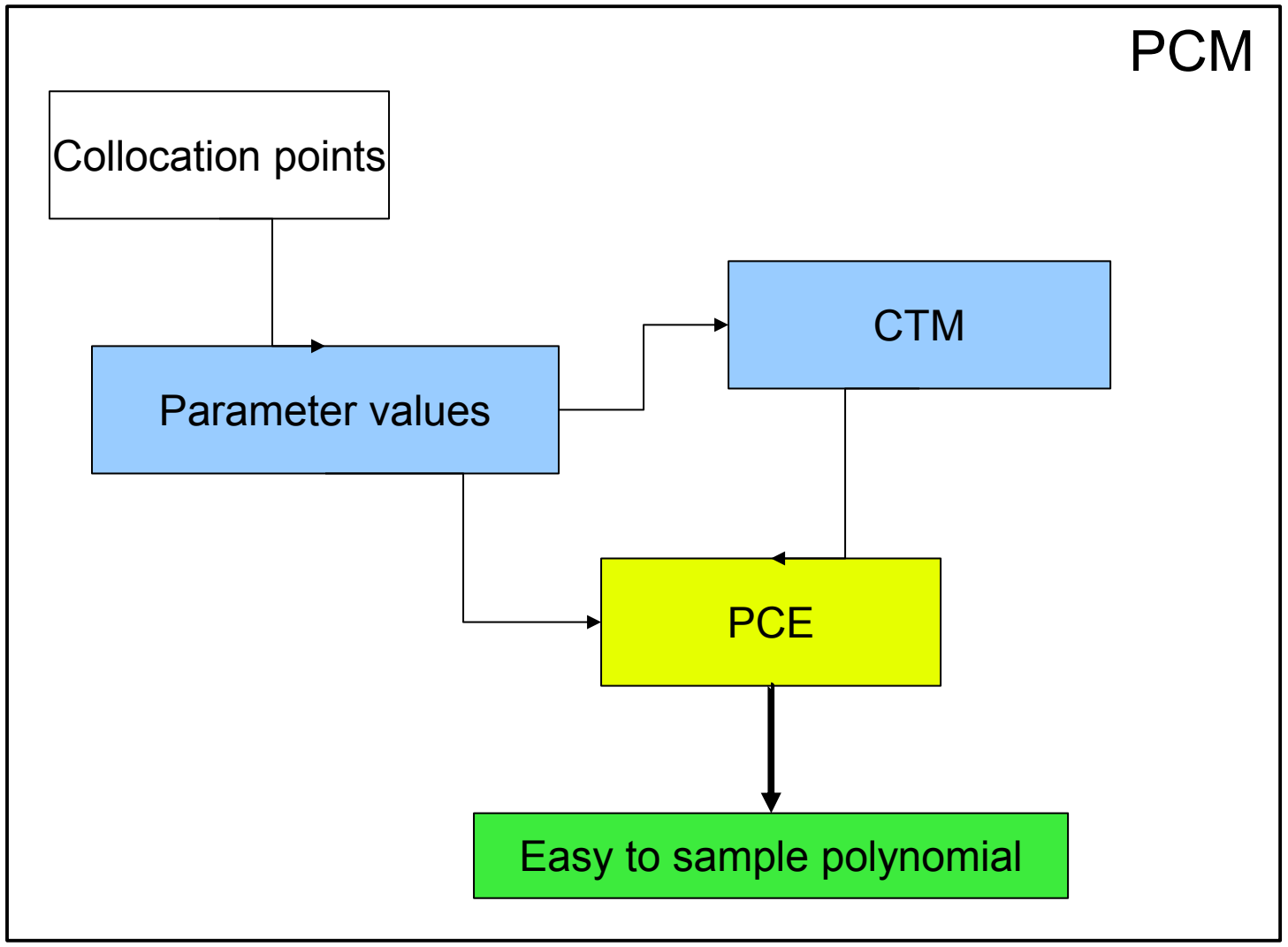
The figure is from
C.L. Friedman and N.E. Selin. 2012. “Long-range atmospheric transport of polycyclic aromatic hydrocarbons: A global 3-D model analysis including evaluation of Arctic sources.” *Environmental Science and Technology*, 46, 9501-9510.

Please see the figure on page:
http://pubs.acs.org/appl/literatum/publisher/achs/journals/content/esthag/2012/esthag.2012.46.issue-17/es301904d/production/images/large/es-2012-01904d_0001.jpeg

The problem

Given the uncertainty of the parameters that affect the outcome of GEOS-Chem's benzo[a]pyrene simulations, what is the resulting uncertainty in Arctic mean total (gas- and particle-phase) atmospheric concentrations?

Uncertain parameters and PCM

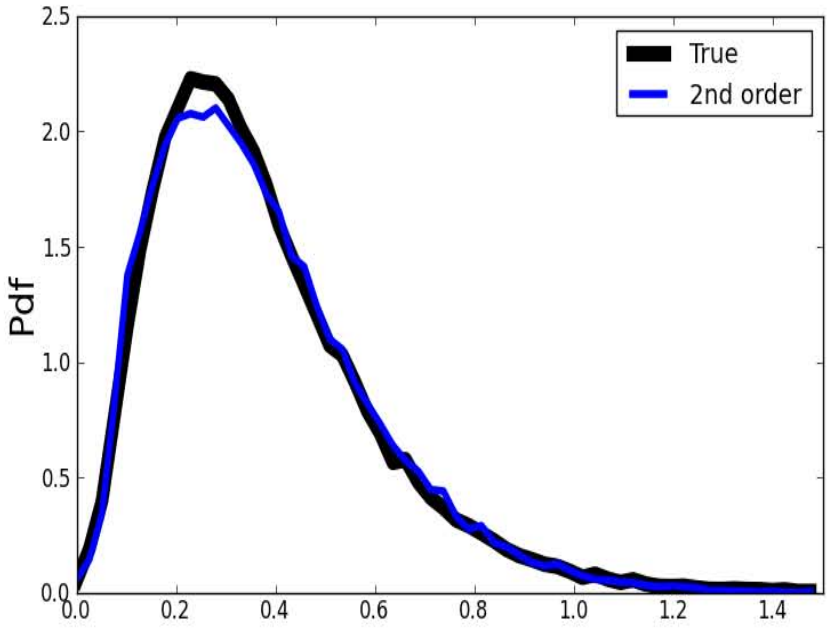


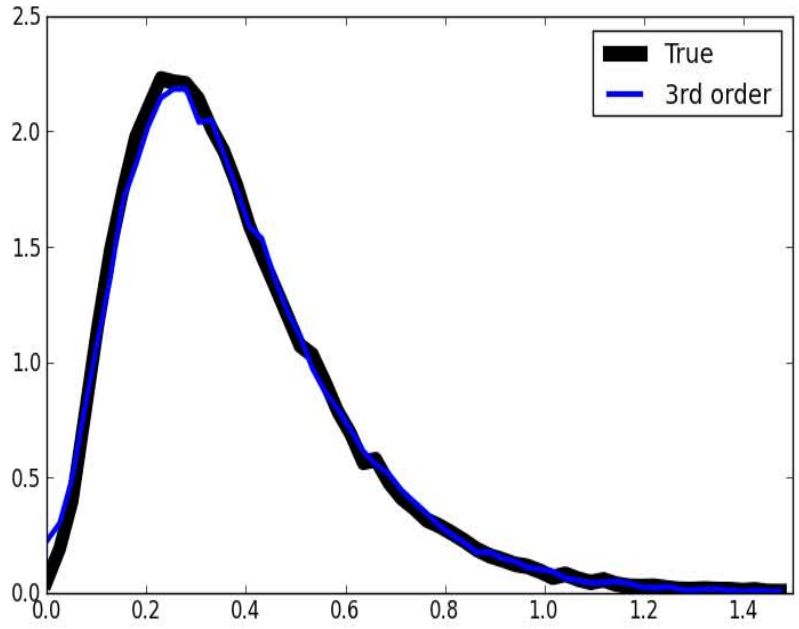
Testing

Test it out with an example from Pan et al.

$$\Delta F = S_0 (1-A_c) T^2 (1-R_s) \beta \delta$$

- Run through PCM scheme to get polynomial estimate
- Compare randomly sampled true function with randomly sampled estimate polynomial


True
2nd order
Pdf
0.0
0.5
1.0
1.5
2.0
2.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4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2.0
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0.2
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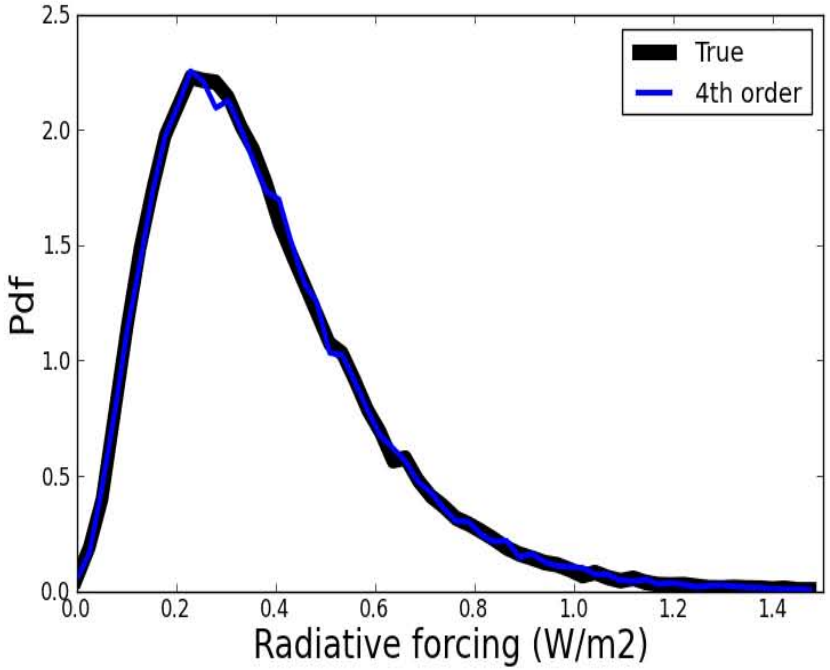
0.6
0.8
1.0
1.2
1.4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4th order
Pdf
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1.5
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2.5
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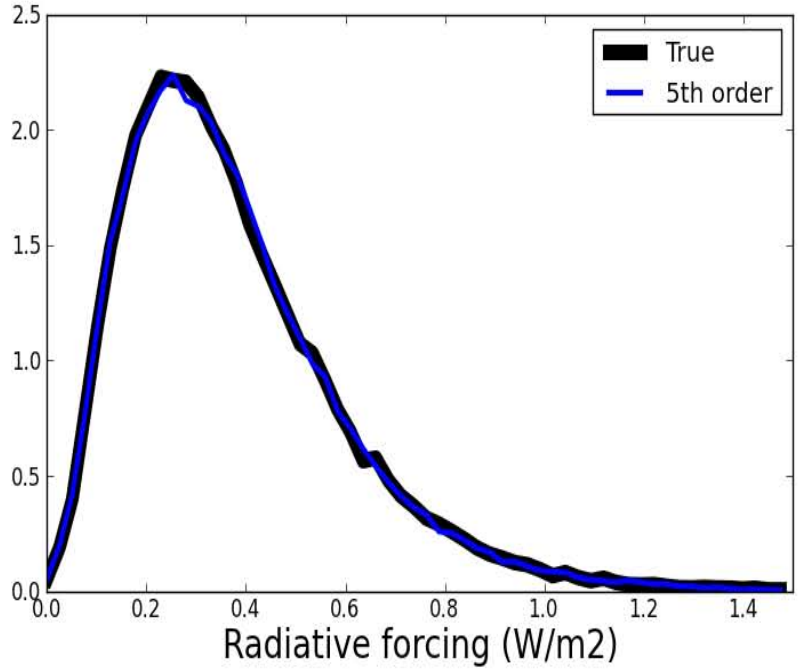
0.6
0.8
1.0
1.2
1.4
Radiative forcing (W/m2)


True
5th order
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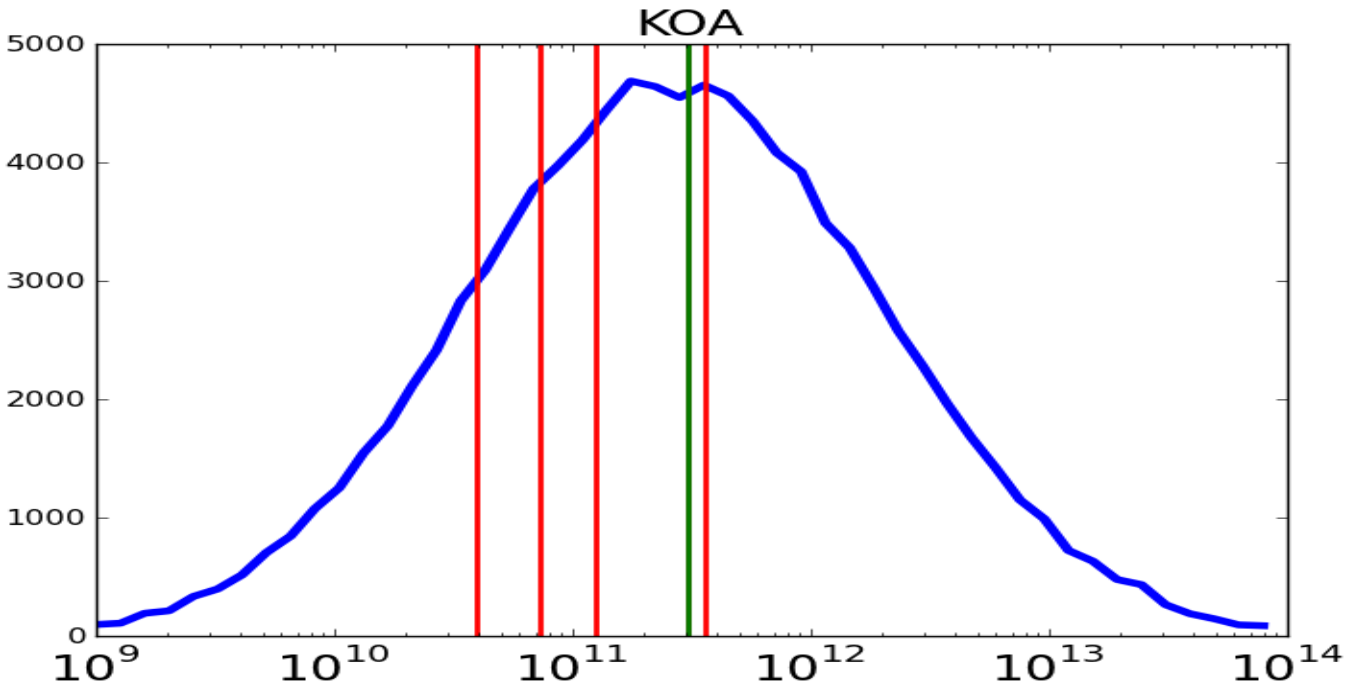
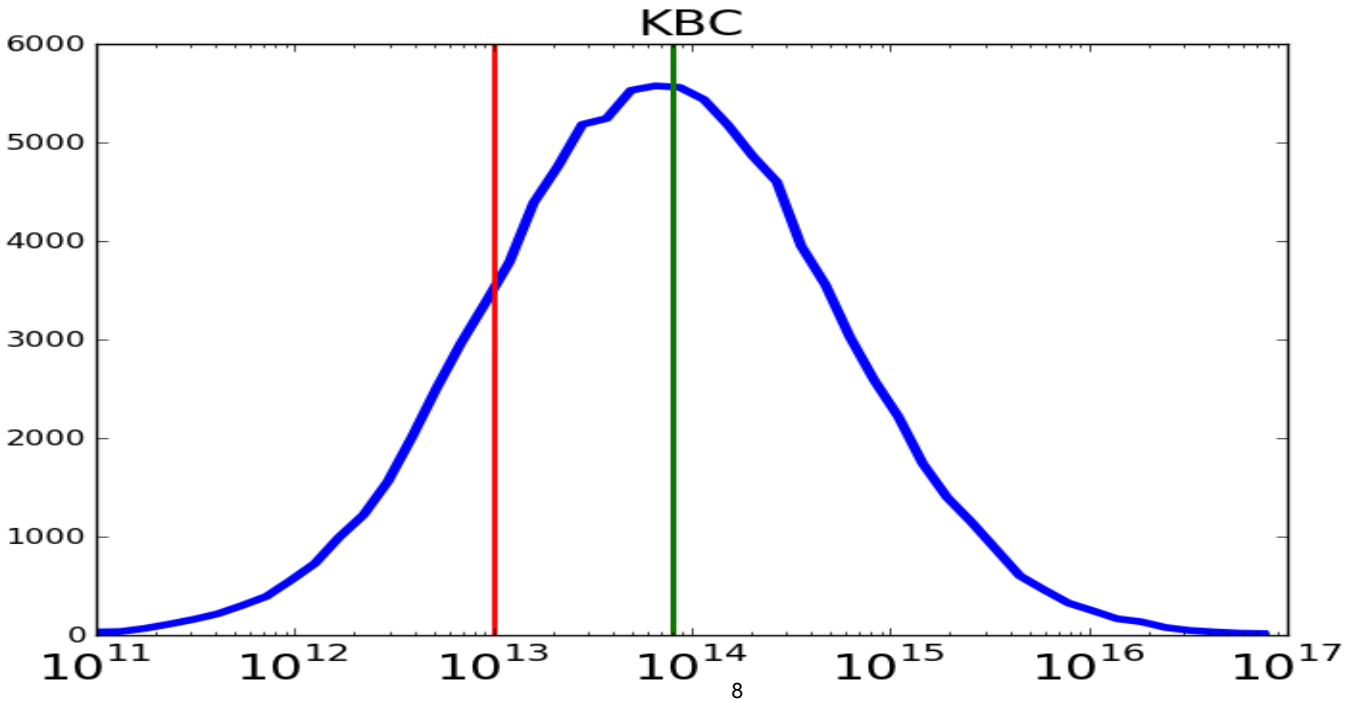
1.0
1.5
2.0
2.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Radiative forcing (W/m2)

Chemical parameters

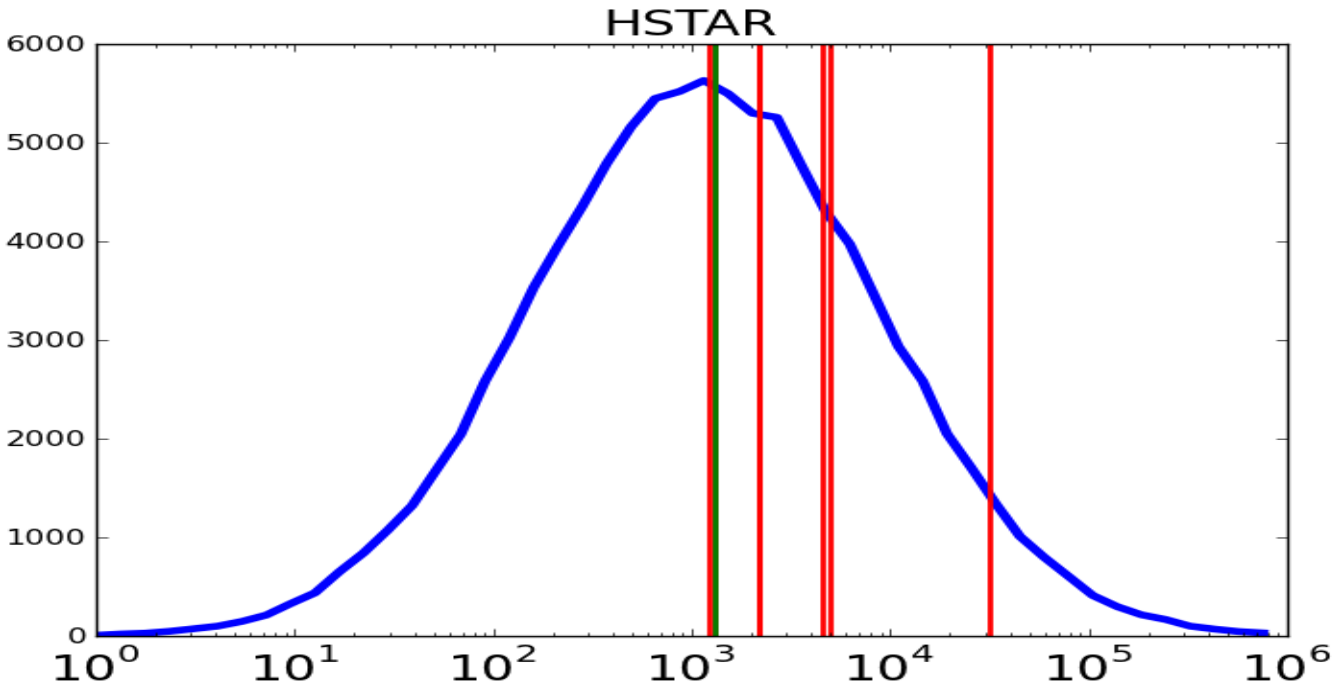
- K_{OA} octanol-air partition coefficient
- K_{BC} black carbon-air partition coefficient
- k_{OH} oxidation rate (by OH^-)
- H* Henry's Law constant
- Δ_H enthalpy of phase transfer (gas to OC)
- Δ_{Hw} enthalpy of phase transfer (gas to aqueous)

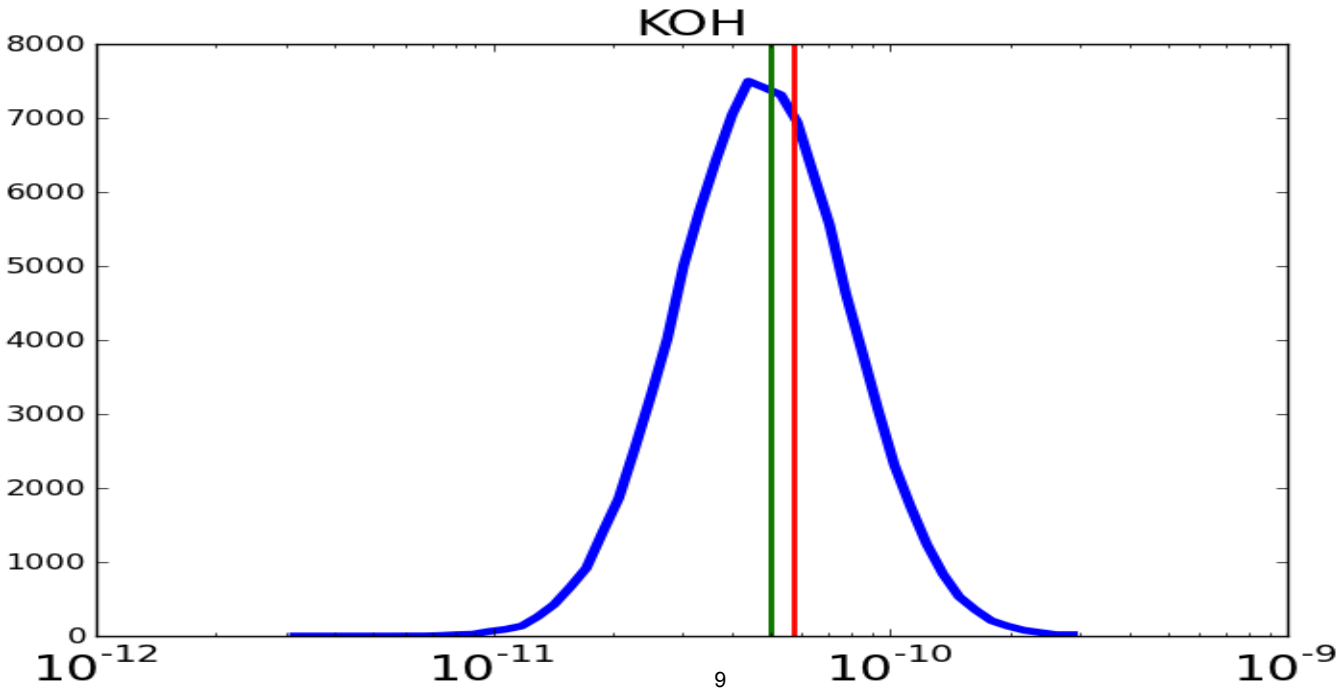
Parameter space



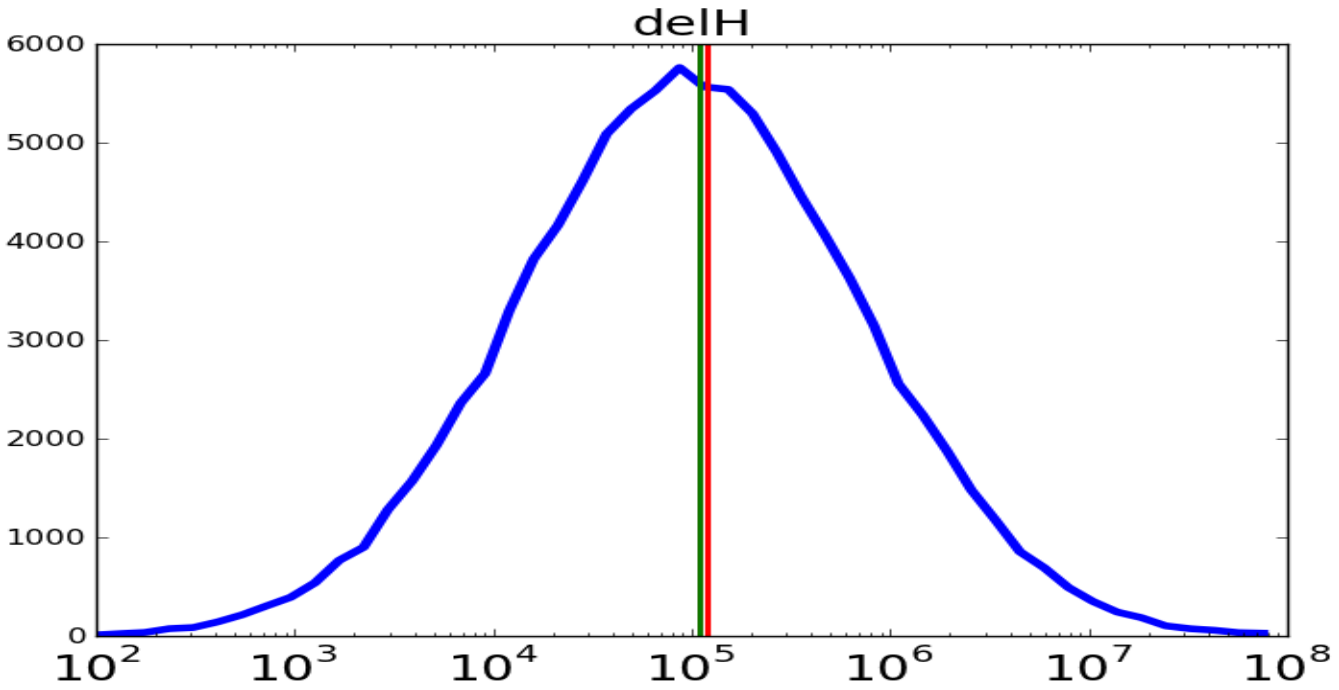


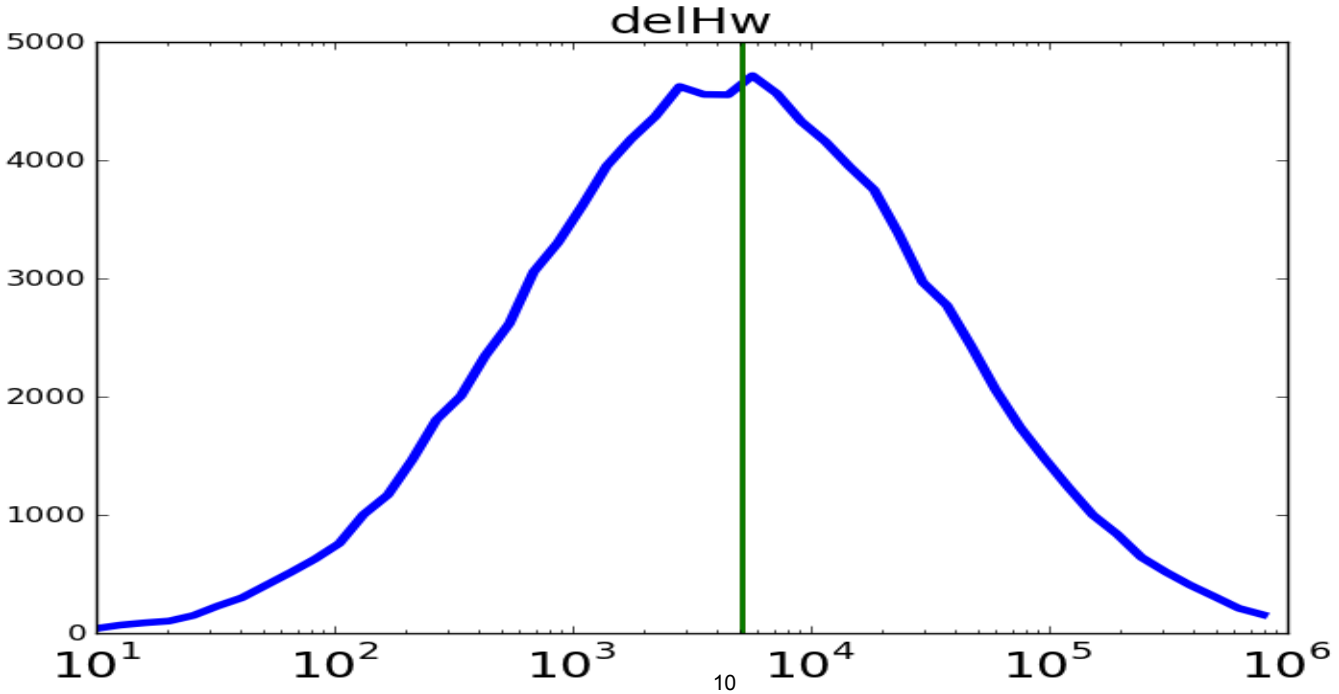
Parameter space





Parameter space

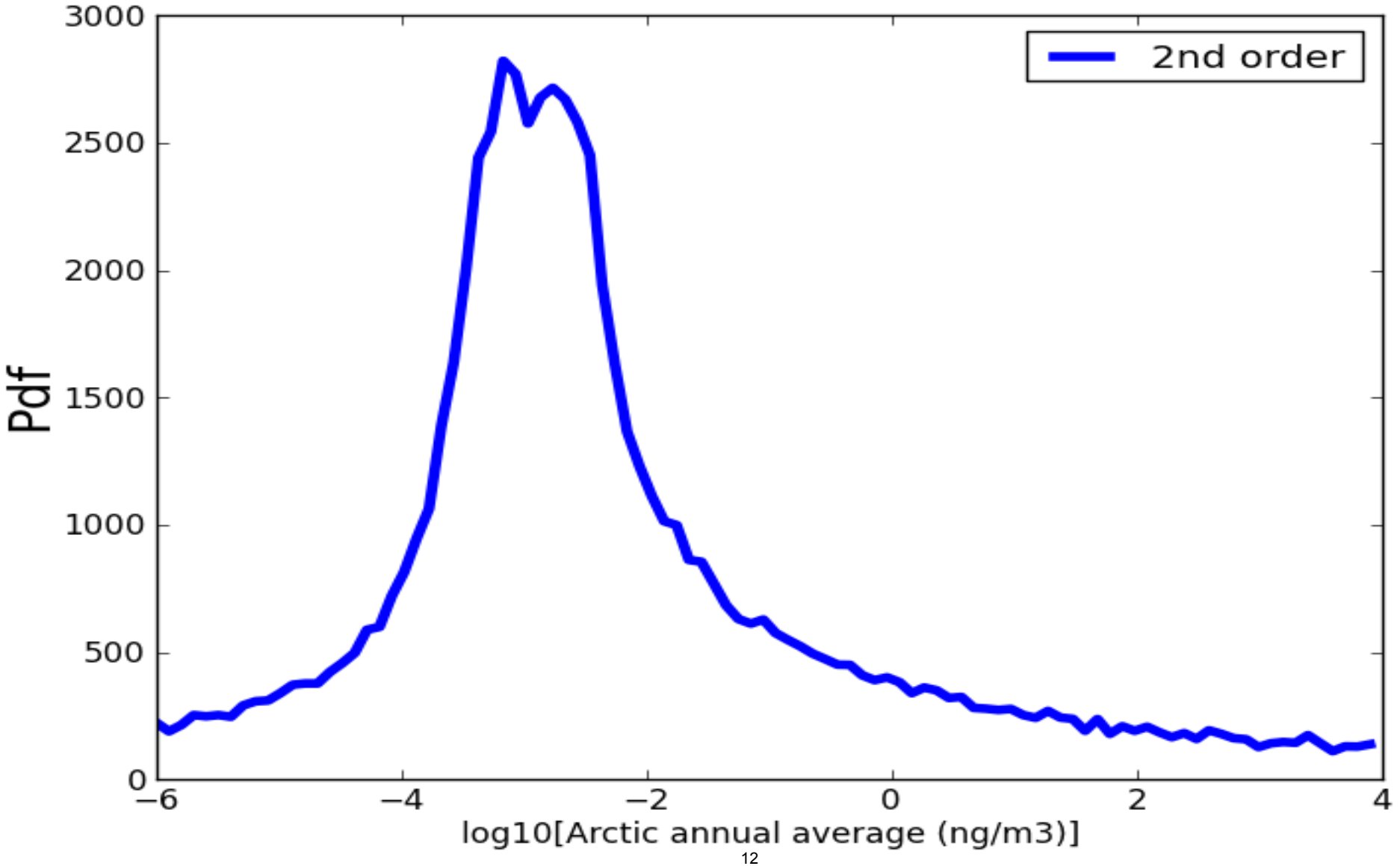




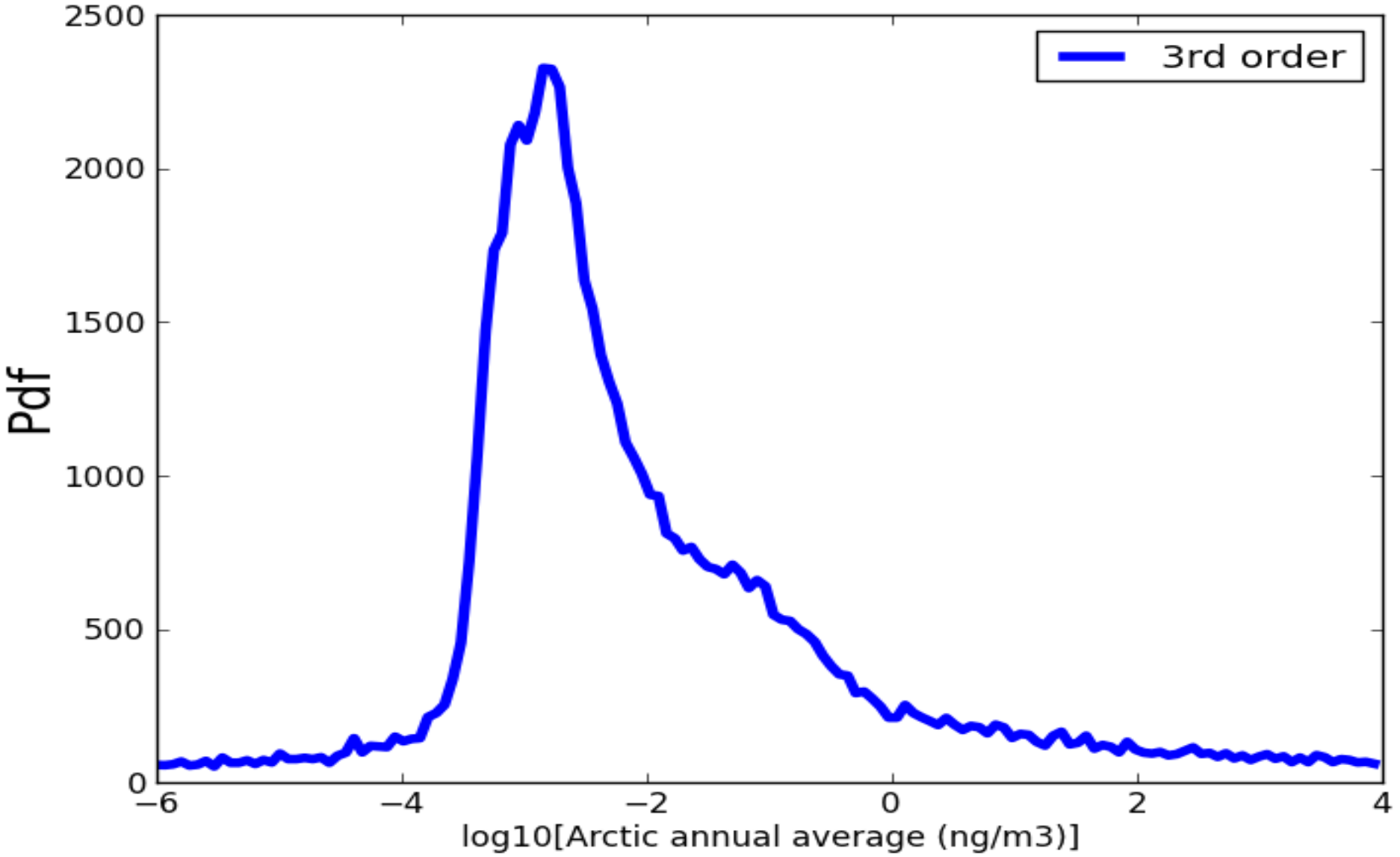
GEOS-Chem model runs

- Prescribed meteorology, emissions
- Benzo[a]pyrene is modeled “offline”
- For each run, parameters are set and a 1 year spin-up is performed, followed by 1 year of simulation
- 112 runs performed (28 + 84)
- Log of resulting concentrations is used

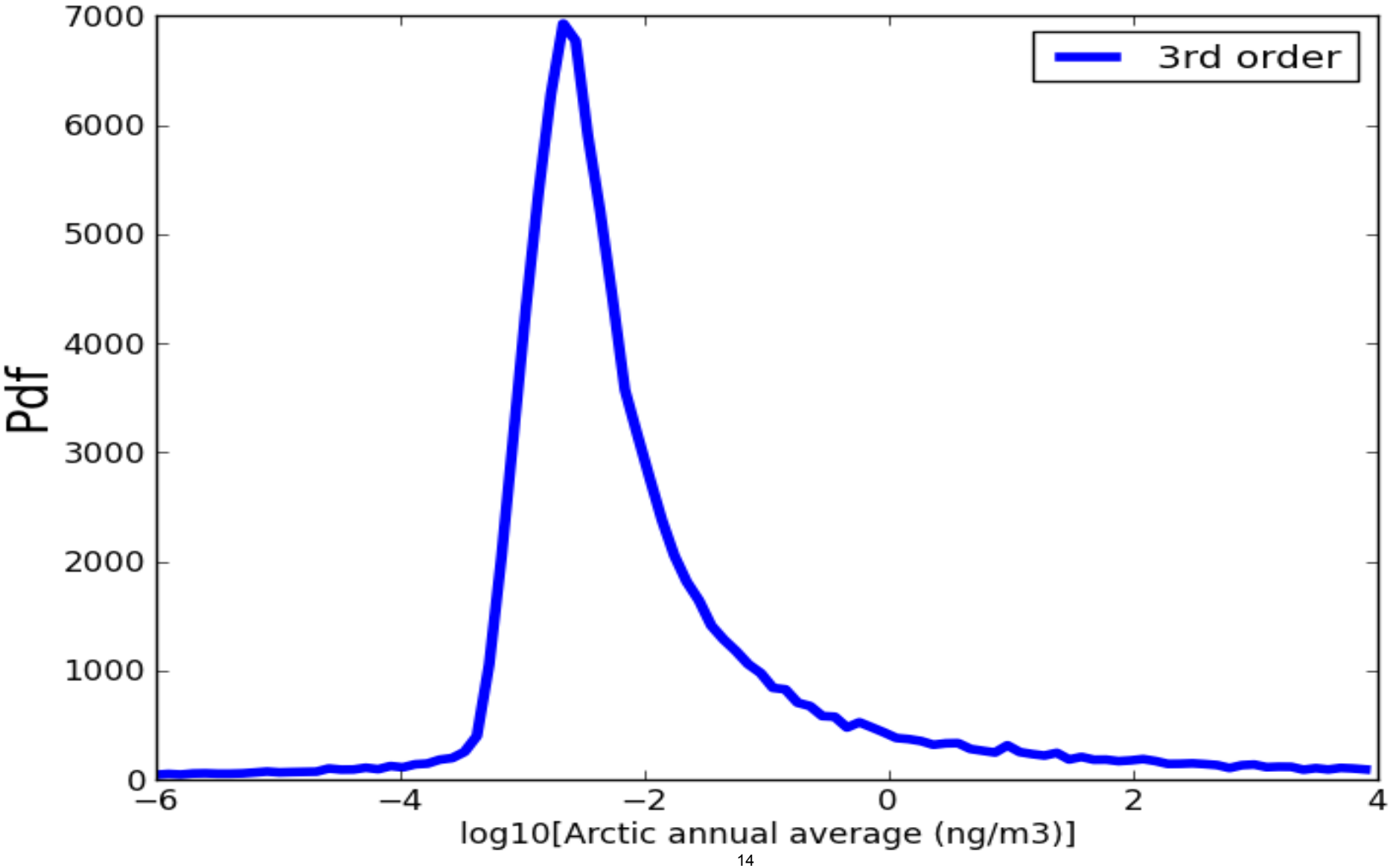
2nd order results



3rd order results



With lower parameter uncertainty



What it means

- PCM gives a reasonable result at low order, even for CTM simulations
- Even given large parameter uncertainty, Arctic concentrations likely in the 0.0003 – 0.01 ng/m^3 range
- More optimistically, 0.001 – 0.01 ng/m^3

What it doesn't mean

- Only includes model response to the given parameters
- Does not include uncertainty due to emissions
- Under the assumption that the chemistry is correct (complete)

Another option

- Regression-based surface response model

- use most of the same procedure, but instead of solving a system of equations (n by n matrix) for the PCE coefficients, use singular value decomposition to get them (m>n by n matrix)

- would provide a good comparison, as a “similar but different” method

- currently under construction

12.S990 Quantifying Uncertainty

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