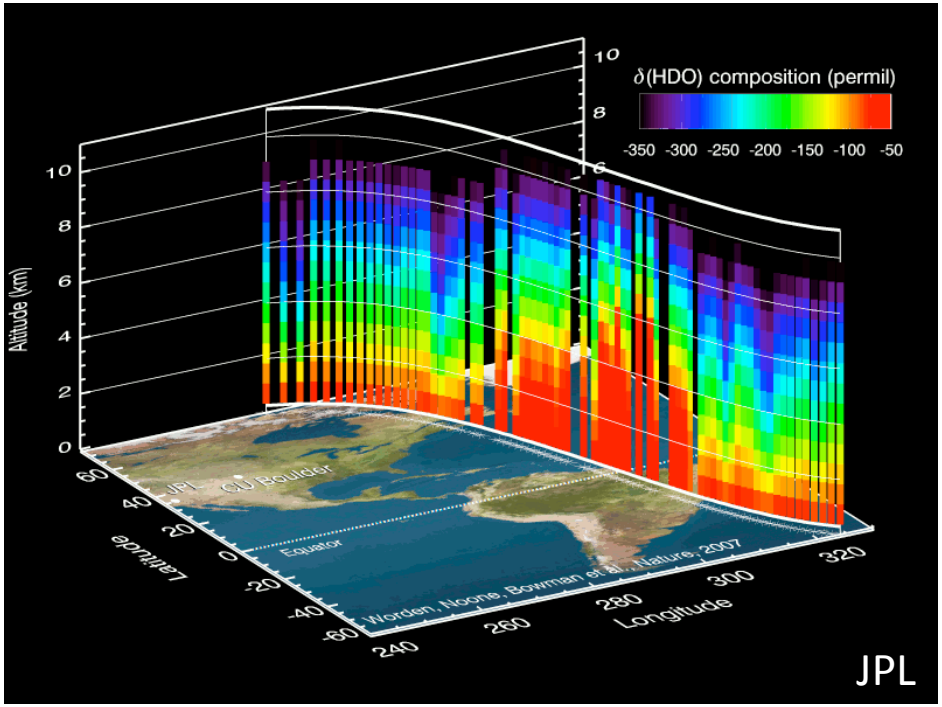
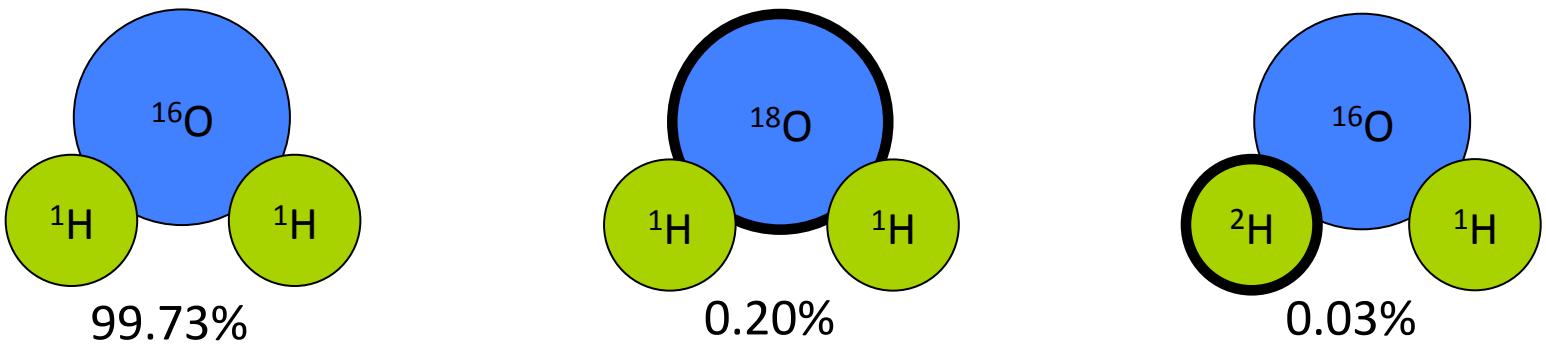
A Tropospheric Emission Spectrometer HDO/H_2O retrieval simulator for climate models



Robert Field, Camille Risi, Gavin Schmidt, John Worden, Apostolos Voulgarakis, Allegra LeGrande, Adam Sobel, Rick Healy

Stable isotopes (isotopologues) of water



There are different isotopes of water, each with a slightly different mass. $H_2{}^{16}O$ is by far the most abundant, but $H_2{}^{18}O$ and HDO exist in measurable quantities.

The heavy isotopes of water evaporate less readily and condense preferentially.

Stable isotopes (isotopologues) of water

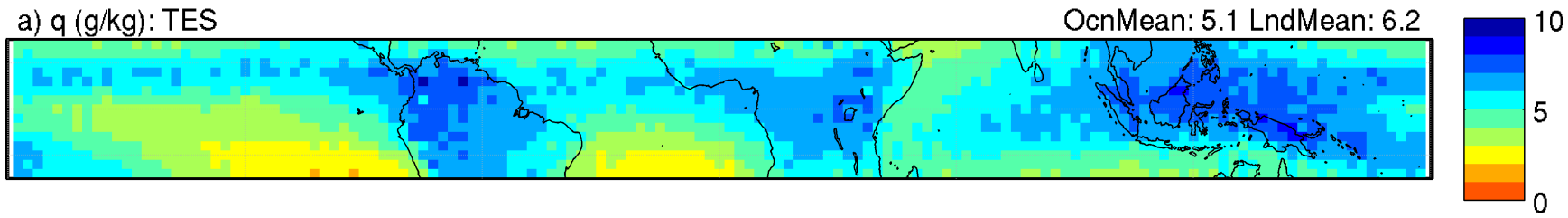
$$R = \frac{[HDO]}{[H_2O]}$$

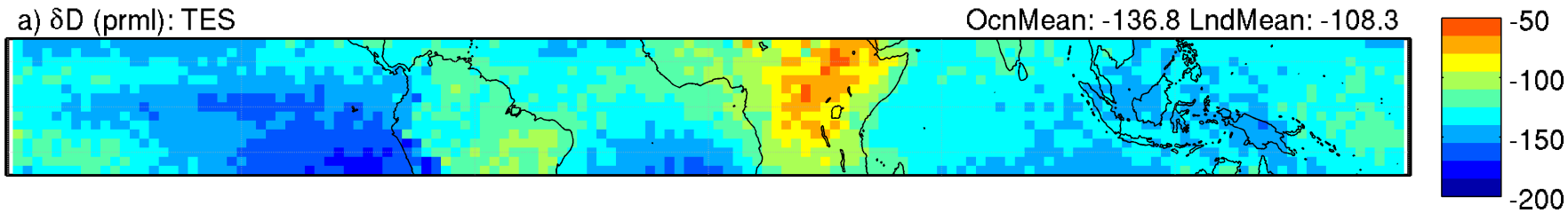
The isotopic composition of a sample is described as a ratio of heavy to light isotope concentrations.

$$\delta D = \left(\frac{R - R_{VSMOW}}{R_{VSMOW}}\right) * 10^3$$

Measurements are usually expressed relative to an ocean water standard, in units of permil (‰).

TES q and δD over 500-800 hPa, 2006-2009

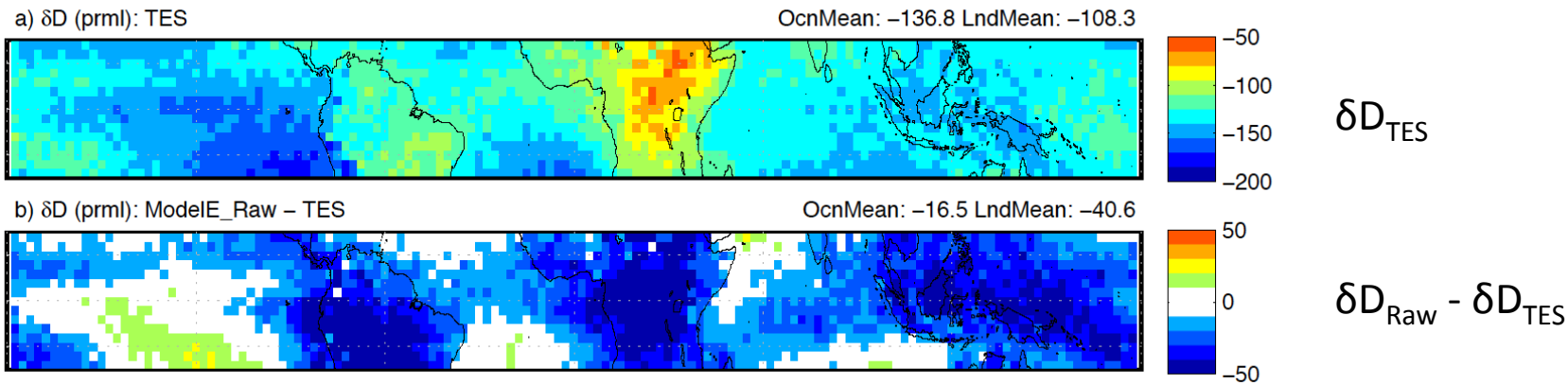




Motivation

- A model must be able to reproduce moisture amount and its isotopic composition.
- Discrepancies in the modeled isotopic composition are more likely due to 'errors' in the the cloud physics than to errors in isotopic physics (which are much simpler).
- There are now sufficient measurements in the troposphere to evaluate models this way:
  - TES: vertical profiles, most sensitive in lower trop.
  - SCIAMACHY: total column, mainly over land
  - ACE-FTS: UT/LS

TES vs. ModelE δD over 500-800 hPa, 2006-2009



The model δD is significantly lower than the TES measurements, especially over land.

However

- Certain features of the satellite retrieval must be taken into account in any quantitative comparison.
- Namely:
  - Model profiles that would be poorly retrieved by the satellite instrument need to be excluded.
  - An instrument operator must be applied to the remaining profiles. This takes into account the vertical sensitivity of the retrieved to actual profile.
- The goal is to produce a new instrument-equivalent model field: **"what would the instrument retrieve if it were flying inside the model?"**

Outline

- Characteristics of the TES HDO/H_2O operator
- The standard approach to applying the operator for prescribed meteorology, and why this may not work in some cases
- A new approach
- Effects of either approach on the modeled HDO/H_2O fields
- Brief comparison with HDO/H_2O observations

Aura TES HDO/H_2O nadir retrieval

- A-train, repeat cycle of 16 days
- HDO/H_2O retrieval based on emission spectra in thermal IR
- The retrieved profiles represent an adjustment from prior H_2O and HDO constraint profiles.
- The adjustment is estimated iteratively to minimize the difference between the measured spectra and that predicted by a forward radiative transfer model using the estimated profiles as input.

TES HDO/H_2O operator

- Using the notation of Worden et al. (2011), the model profile of HDO/H_2O ratio $\hat{x}_R$ suitable for comparison with satellite measurements is expressed as:

Prior isotopic ratio

Raw model amount profiles

New model isotopic ratio

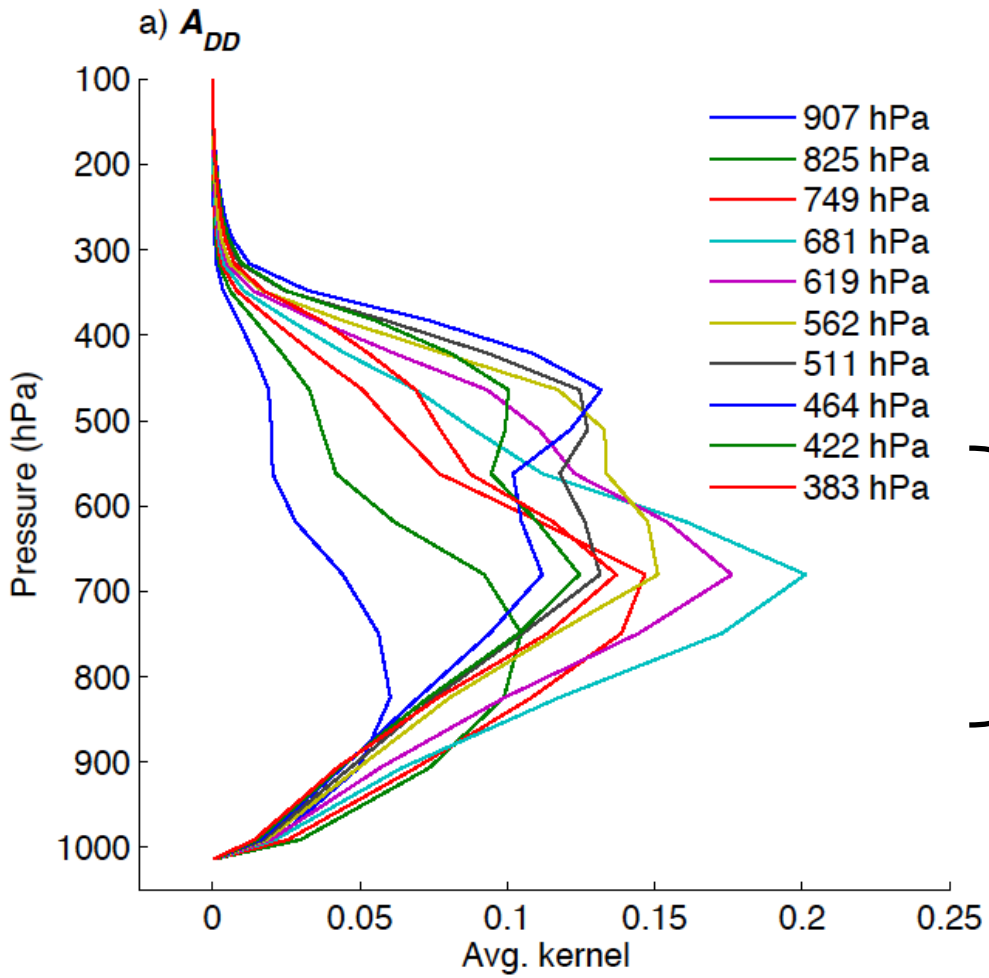
$$\hat{x}_R = x_a^R + (A_{DD} - A_{HD})(x_D - x_a^D) - (A_{HH} - A_{DH})(x_H - x_a^H)$$

Averaging kernels from radiative transfer model

Prior amount profiles

- The averaging kernel matrices represent the sensitivity of the retrieved profile to the actual profile.
- Suitable averaging kernels and H_2O priors must be chosen each time the TES operator is applied.

Example HDO averaging kernel rows



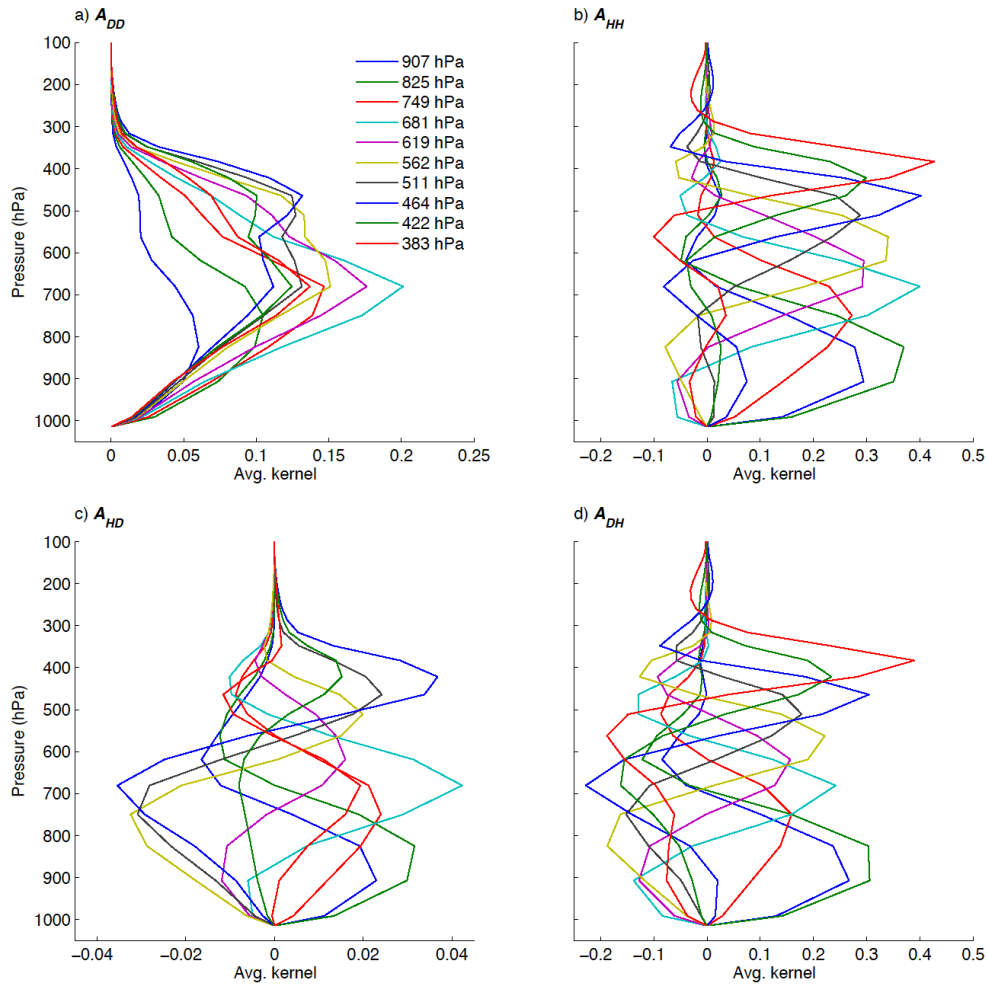
Peak sensitivity is near 700 hPa

We adopt the pressure of peak sensitivity (p_D) as the defining averaging kernel characteristic

Example averaging kernels

Important

Small

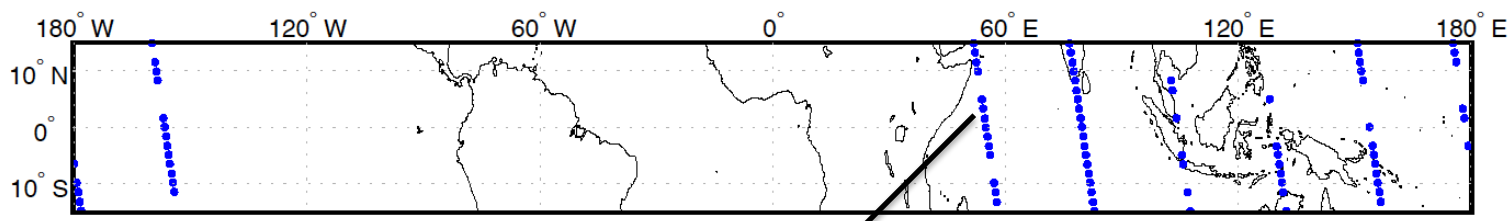


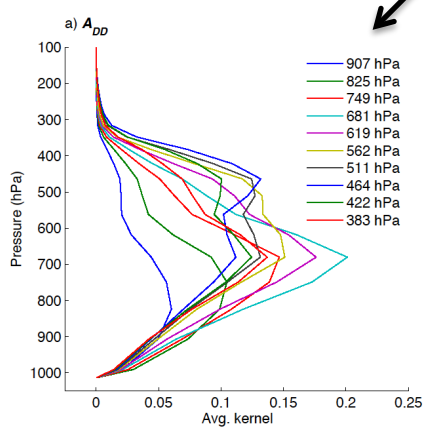
Cancel each other out

Applying the TES operator

- The standard approach is to:
  - sample the model fields at individual measurement points
  - skip the poor quality retrievals
  - for those remaining, use the averaging kernels from individual measurements

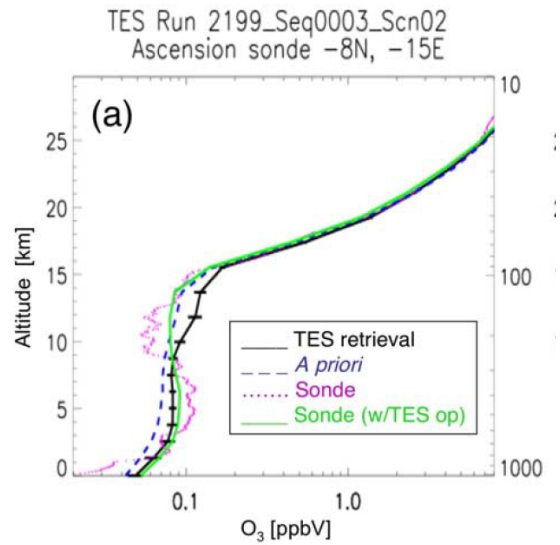
TES sampling on 9 December, 2006 for daytime, high-quality retrievals only





Applying the TES operator

- This approach assumes that there is agreement between the satellite and model in the conditions which influence retrieval quality and averaging kernel structure

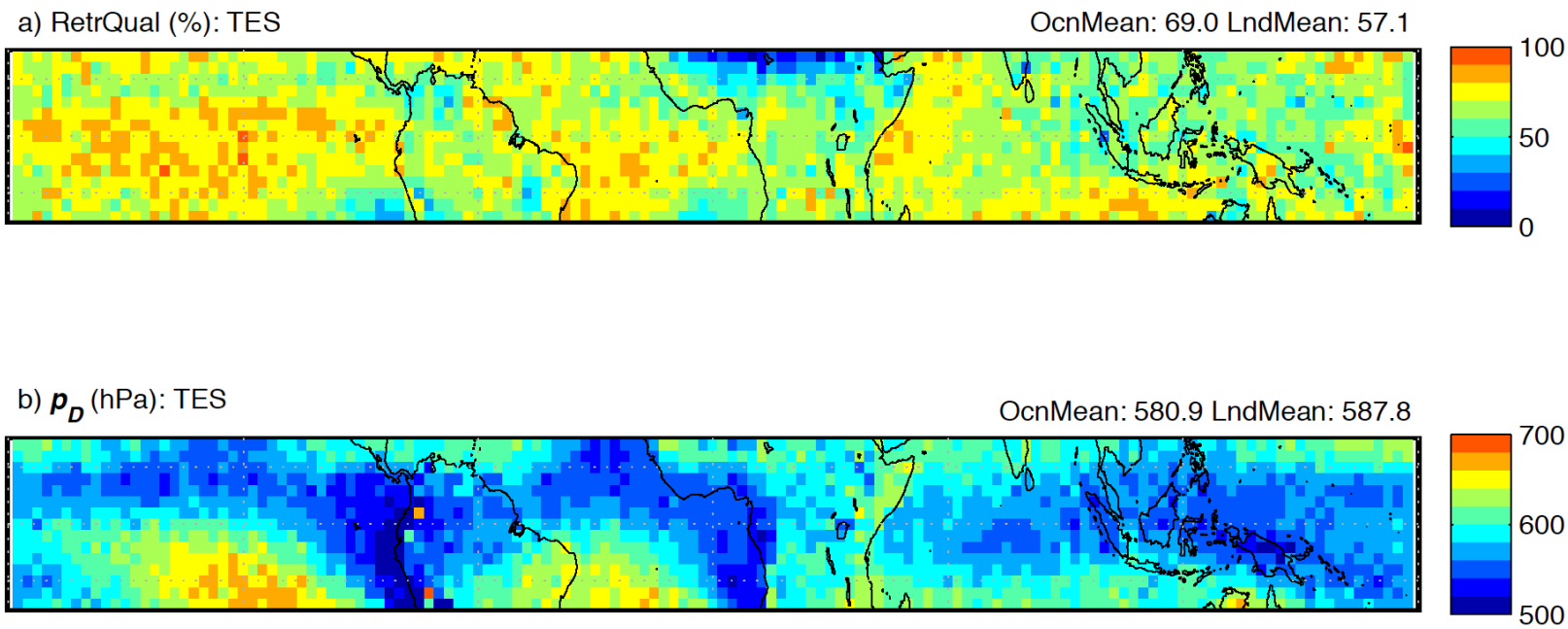


Worden et al. (2007, JGR)

- But what if they do not? For a free-running atmosphere, there is no expectation that they will at short time scales.

- We have tried to develop an approach that predicts, empirically, retrieval quality and averaging kernel structure from model conditions, rather than relying on collocated satellite measurements.

Retrieval quality and p_D from observations



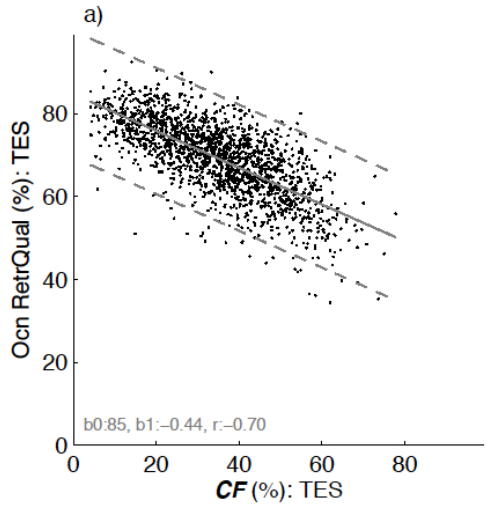
Controls on retrieval quality and p_D

Pattern correlation with underlying meteorological fields

		Retrieval quality		Pressure of peak HDO sensitivity (p_D)	
Description	Variable	Ocean	Land	Ocean	Land
Cloud optical depth	τ	−0.38	0.30	−0.39	−0.35
Cloud fraction (%)	CF	**-0.70**	0.39	−0.55	−0.28
Cloud top pressure (hPa)	CTP	0.33	0.15	0.13	0.00
Prcp. water in bdy. layer (mm)	PW_B	−0.15	0.57	−0.29	−0.39
Prcp. water in free. atm. (mm)	PW_F	−0.43	0.32	**-0.70**	−0.50
Prcp. water total (mm)	PW_T	−0.35	0.44	−0.58	−0.48
Surface temperature (K)	T_S	−0.28	**-0.72**	0.04	**0.51**

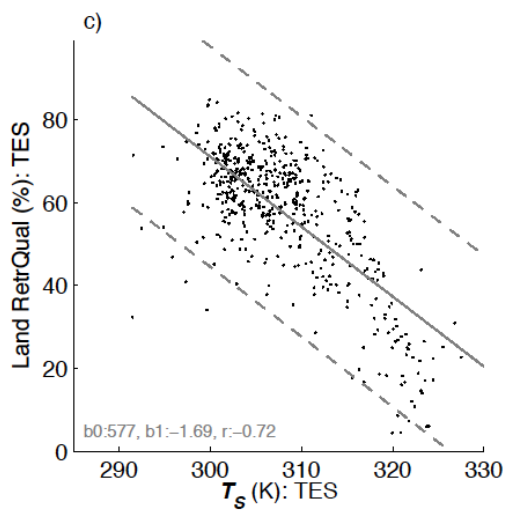
Controls on retrieval quality in observations

Ocean



Retrieval quality over the ocean decreases most strongly with increasing cloud cover

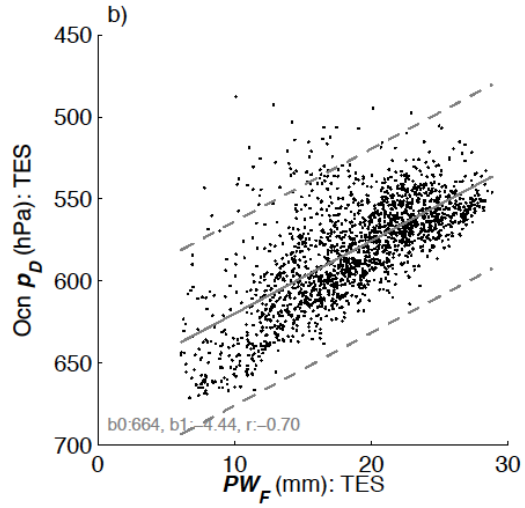
Land



Retrieval quality over land decreases most strongly with surface temperature

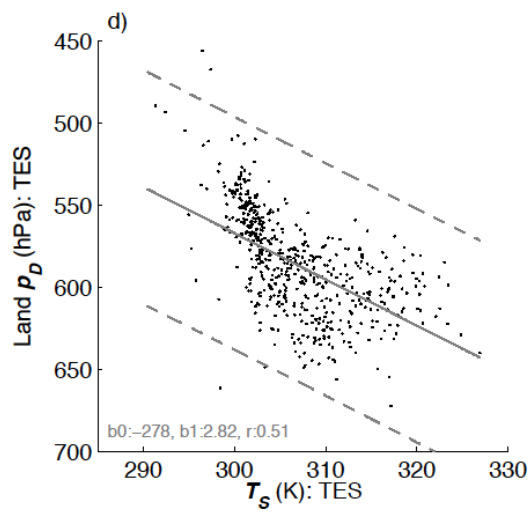
Controls on p_D in observations

Ocean



p_D over the ocean moves closer to the surface with decreasing mid-tropospheric moisture

Land



p_D over the land moves closer to the surface with increasing temperature

ModelE configuration

- AR5 version run from 2006-2009
- Prescribed, monthly-varying SSTs and sea-ice
- Horizontal winds nudged to NCEP/NCAR reanalysis
- TES operator applied 'in-line' using both the standard and new approaches
- See TES_SIMULATOR.f & TRACER_PRT.f

Big lookup tables

The TES observations were binned using the variables that influenced retrieval quality and AK structure

Identifier	Description	Category ranges
LO	Land/ocean	
C	τ	$0, 0.3, 1.3, 3.6, 23, > 23$
	CTP (hPa)	$0, 440, 680, > 680$
C_{fine}	τ	$0, 0.3, 1.3, 3.6, 9.4, 23, 60, > 60$
	CTP (hPa)	$0, 180, 310, 440, 560, 680, 800, > 800$
T	T_S (K)	$< 295, 295, 300, 305, 310, 315, > 315$
PW	PW_B, PW_F (mm)	$0, 10, 20, > 20$
PW_{fine}	PW_B, PW_F (mm)	$0, 5, 10, 15, 20, 25, 30, > 30$

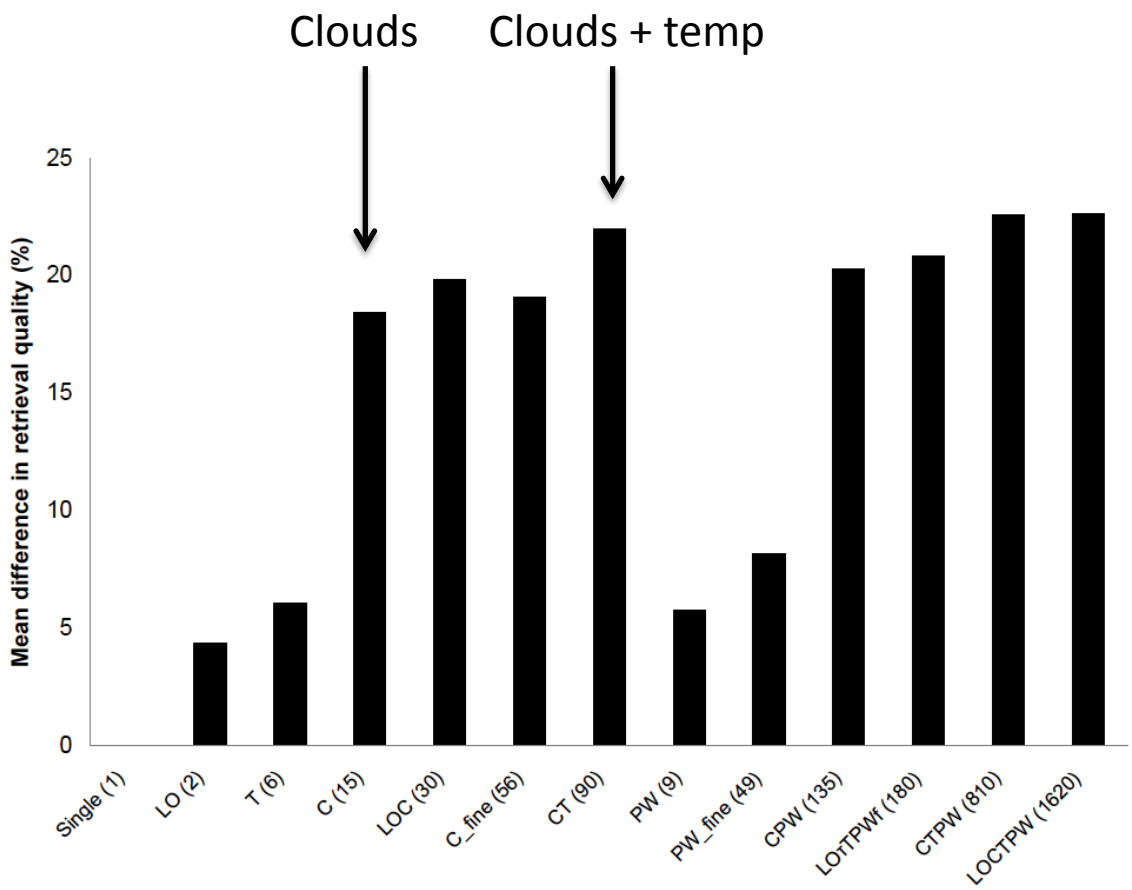
How it works

At each model time step and location along the satellite's orbital path:

- Sample the modeled categorical variable fields (T_{surf}, clouds, precipitable water) in the model
- Look up the associated category from the TES observations
- Include the model profile with probability equal to the category's retrieval quality
- If included, apply the instrument operator using the mean averaging kernels and H_2O priors from that category.

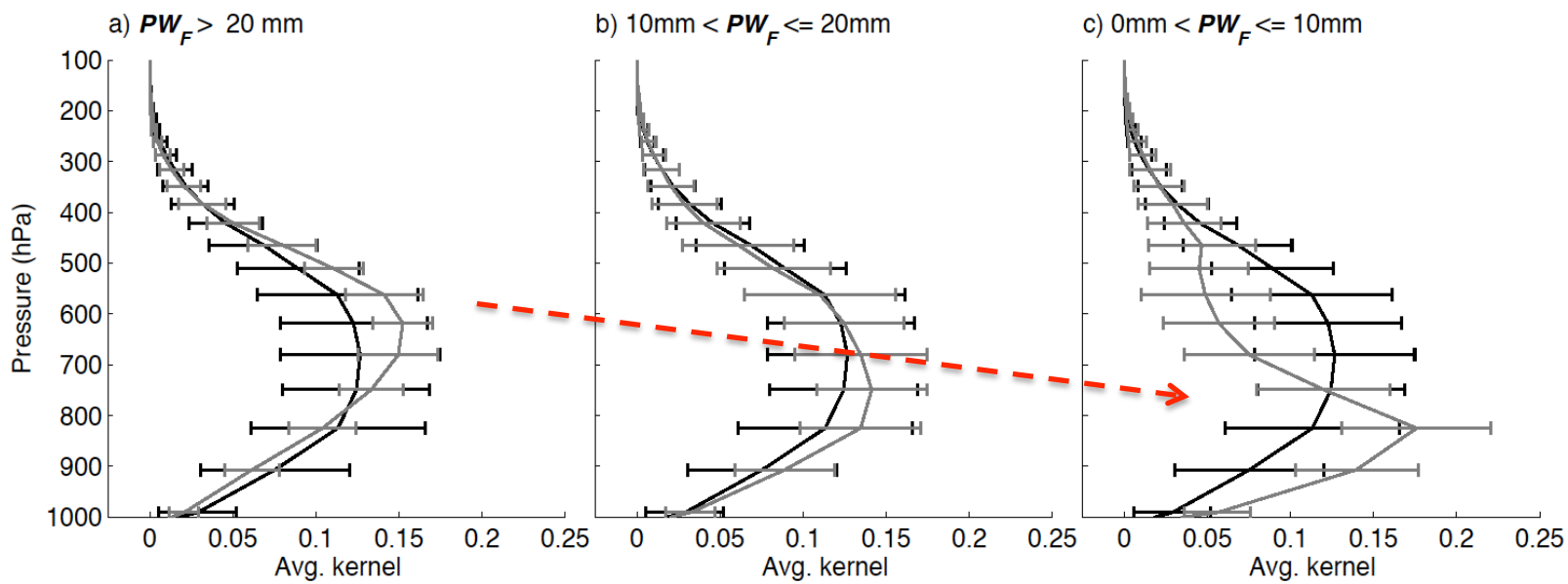
Separation of retrieval quality

How different, on average, is the retrieval quality within different categories from the overall mean?



Example mean averaging kernels

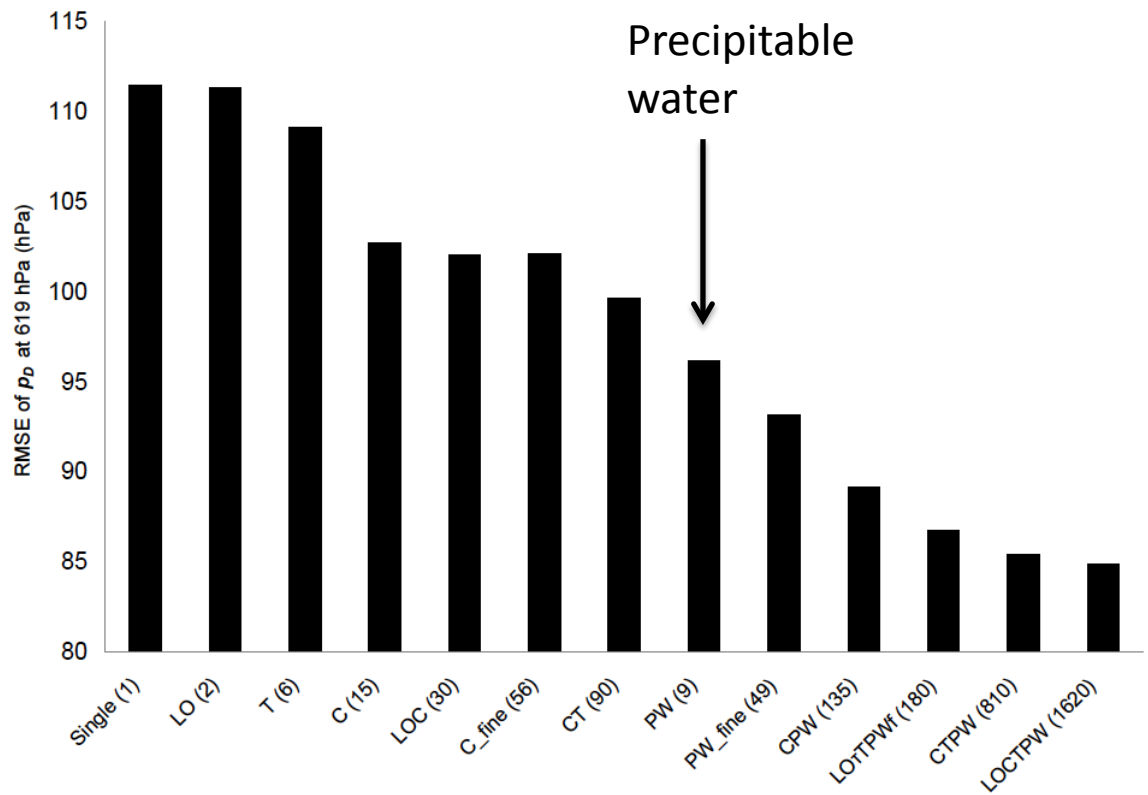
Clear sky averaging kernel rows at 619 hPa for decreasing free-tropospheric moisture



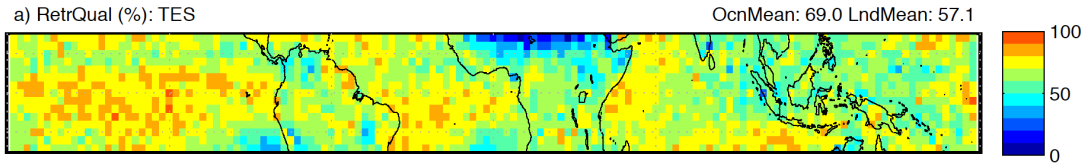
As free-tropospheric moisture decreases, the mid-tropospheric retrievals become more sensitive to boundary layer HDO/H_2O composition

Separation of p_D

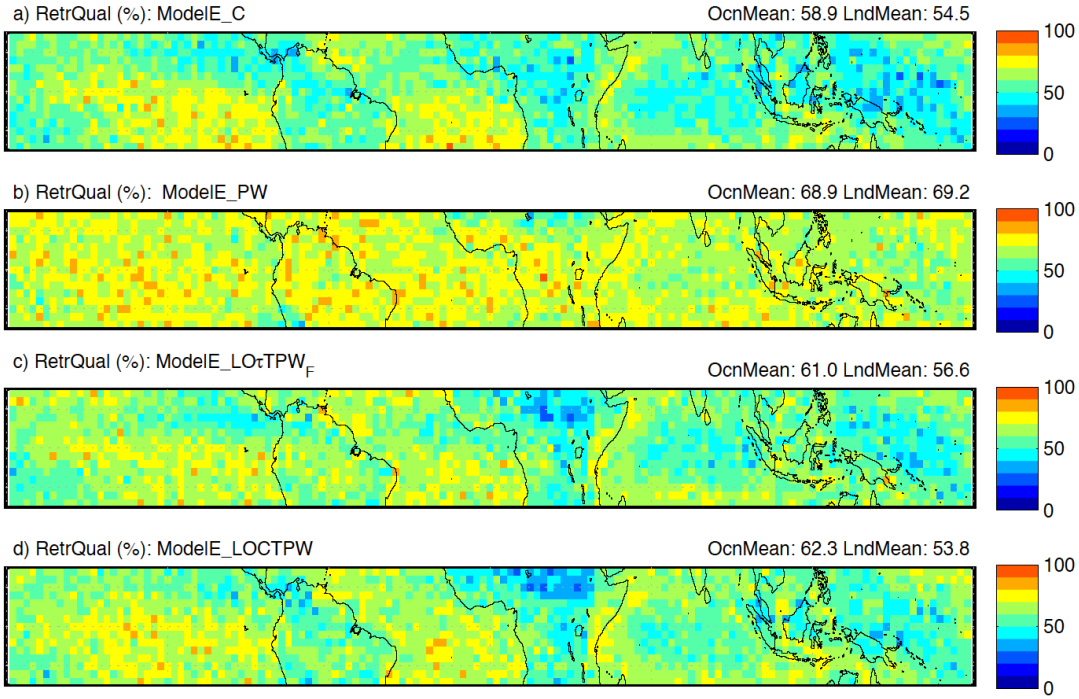
How does the total within-group p_D variance vary within different categories?



Predicted retrieval quality



Obs.



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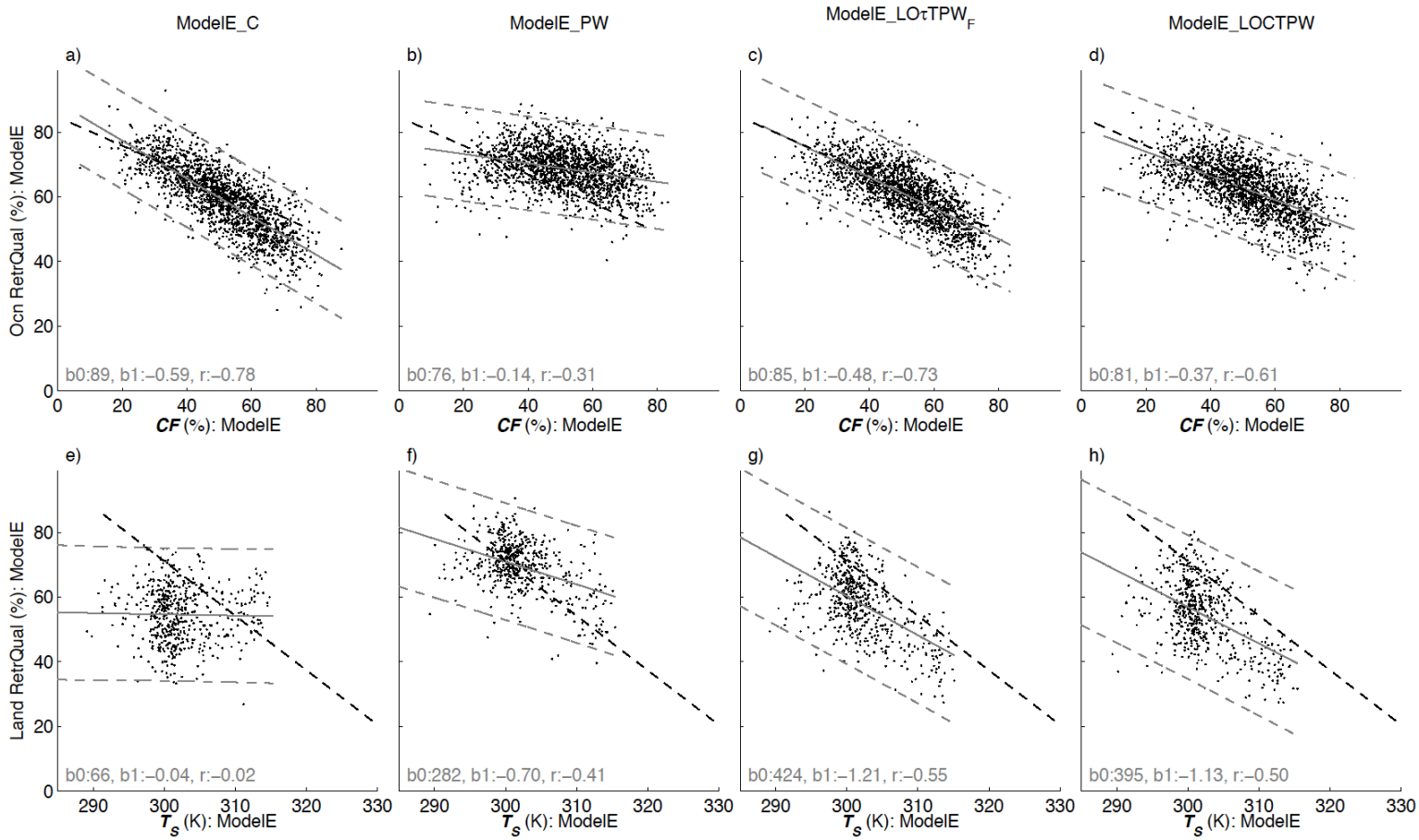
More complicated categorizations

Predicted controls on retrieval quality

*

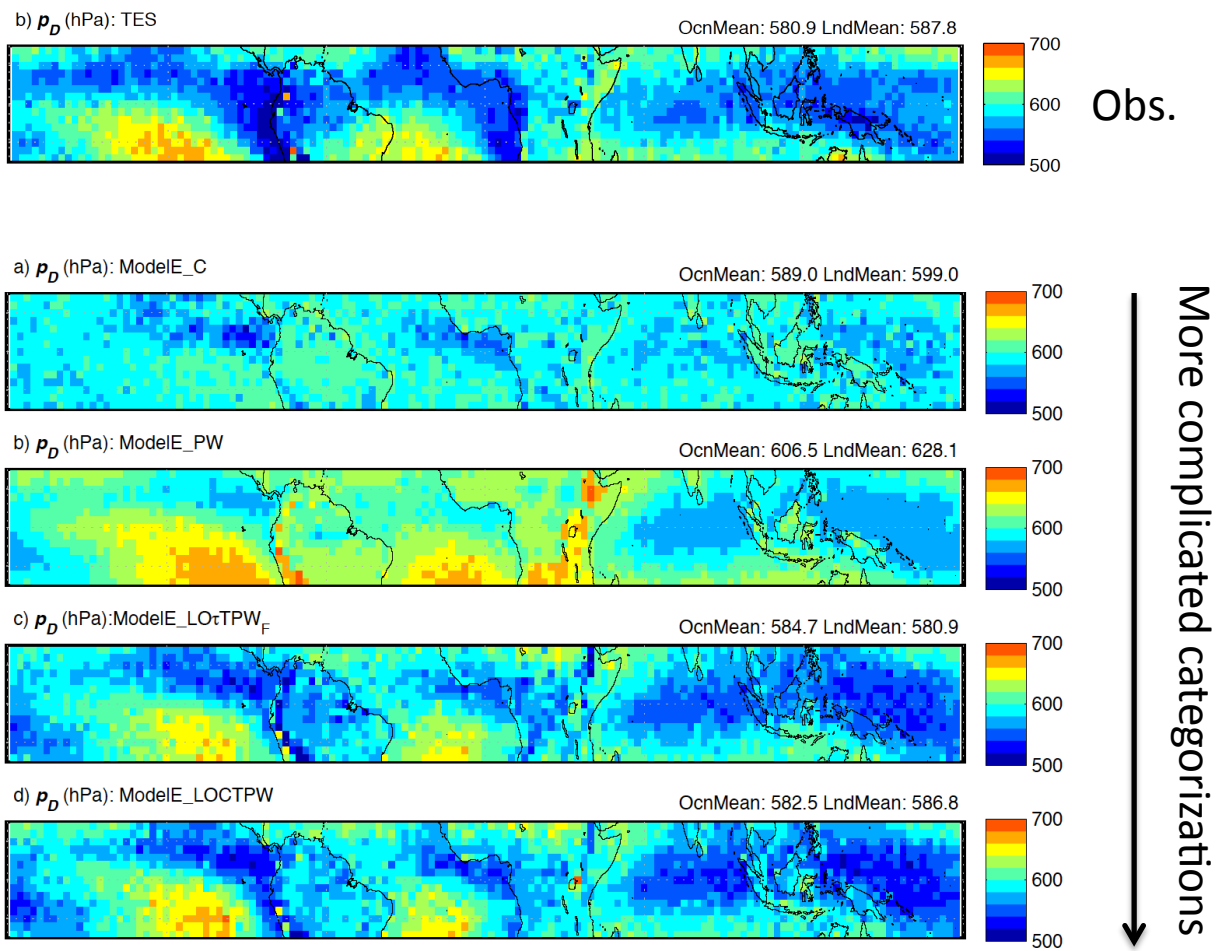
Ocean

Land



Black dashed lines show regression lines from observations

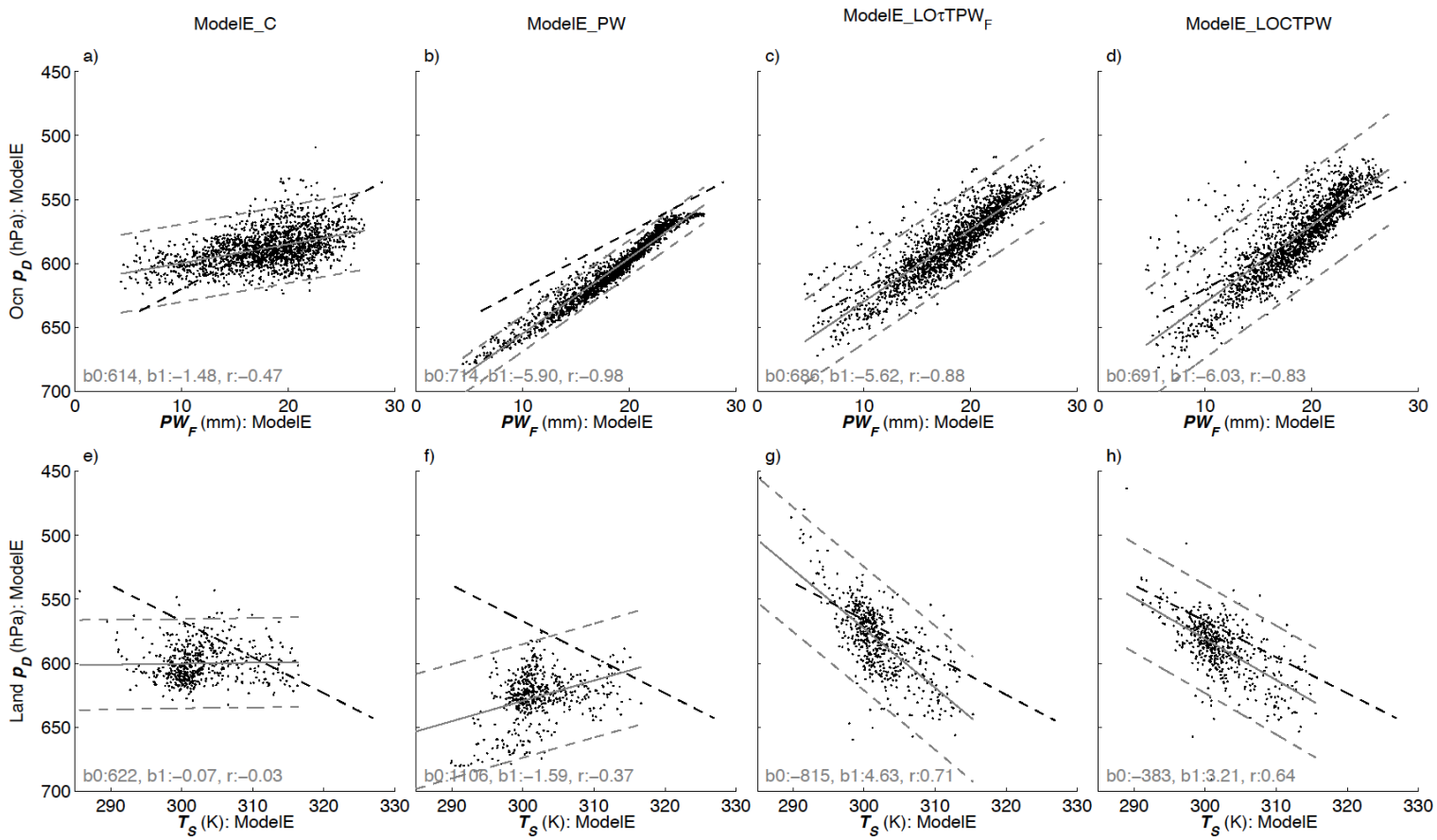
Predicted p_D



Predicted controls on p_D

Ocean

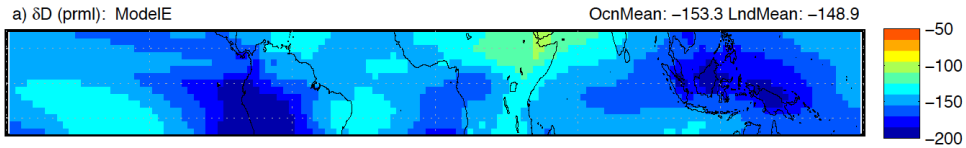
Land



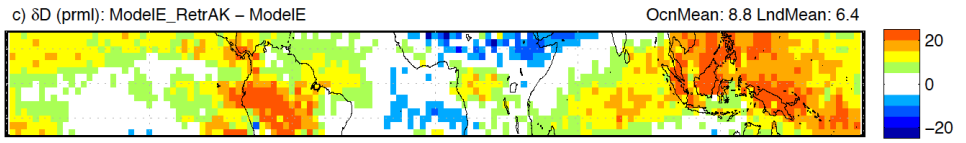
Black dashed lines show regression lines from observations

Effects of TES operator on modeled δD fields

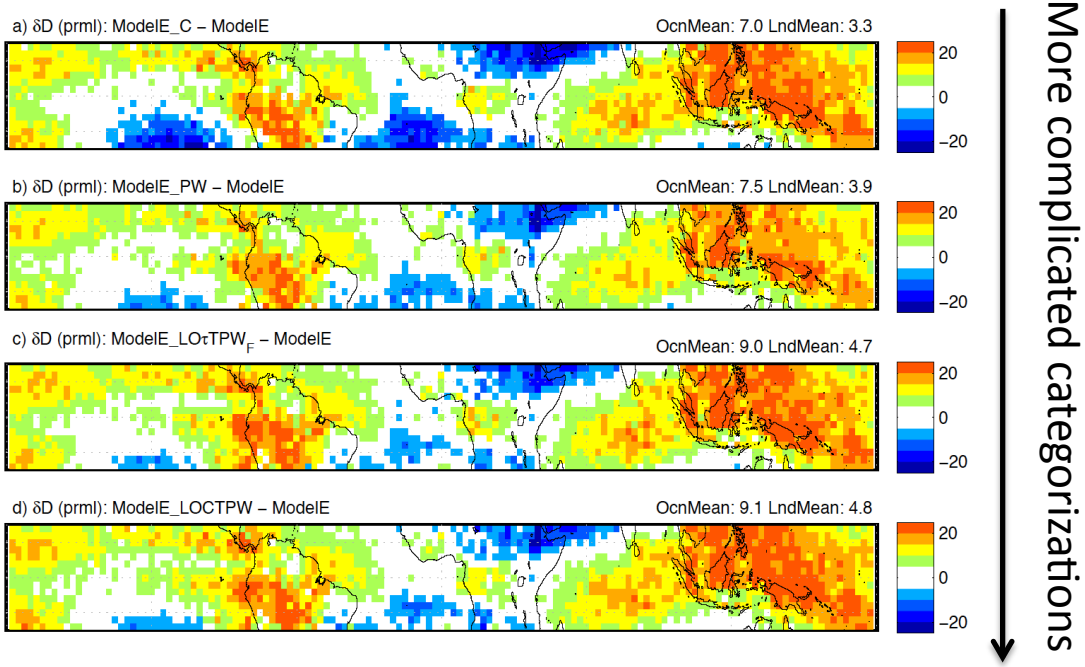
δD_{Raw}



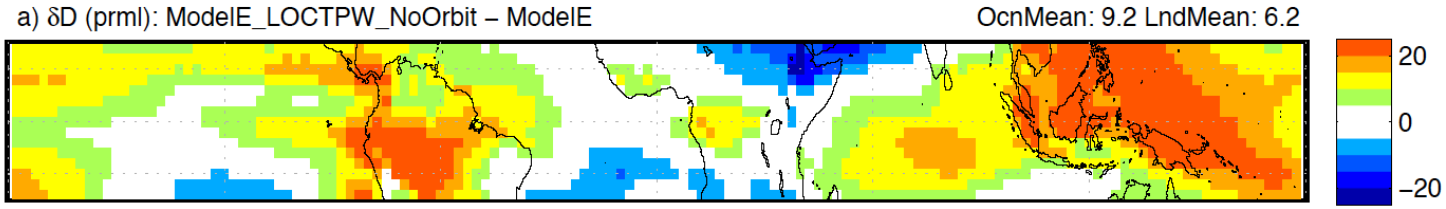
$\delta D_{RetrAK} - \delta D_{Raw}$



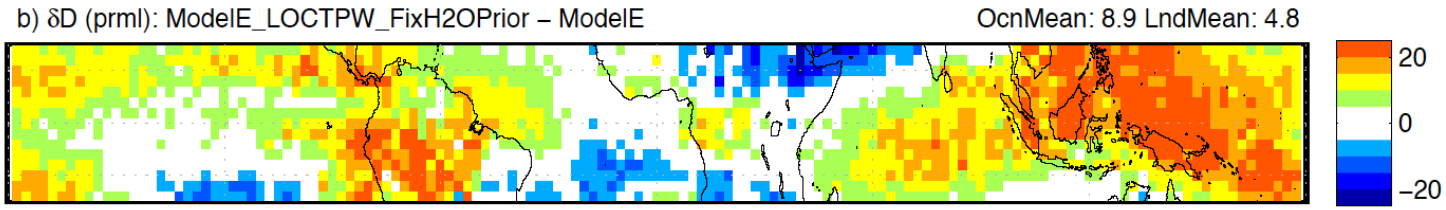
$\delta D_{CatAK} - \delta D_{Raw}$



Sensitivity tests



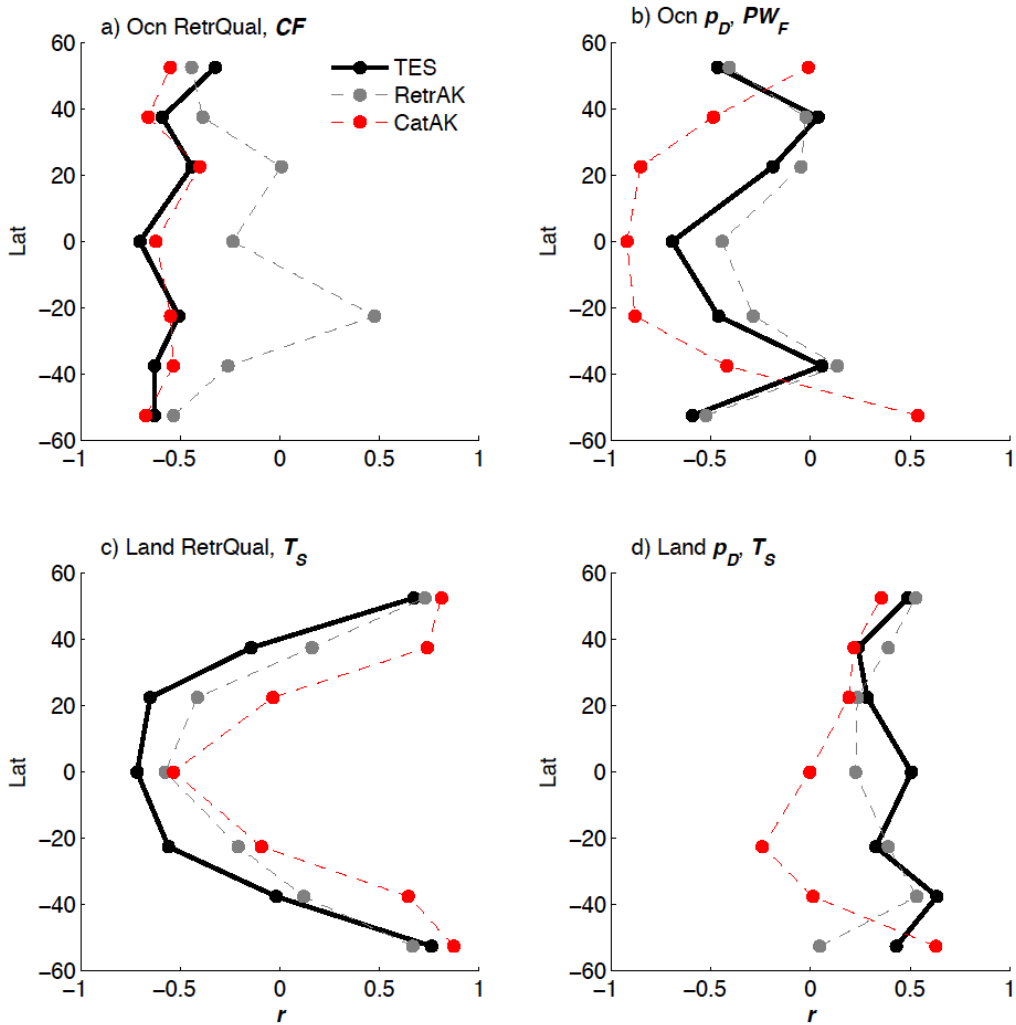
Orbital path sampling: except for more smooth fields, operator insensitive to effects of orbital sampling (over four years)



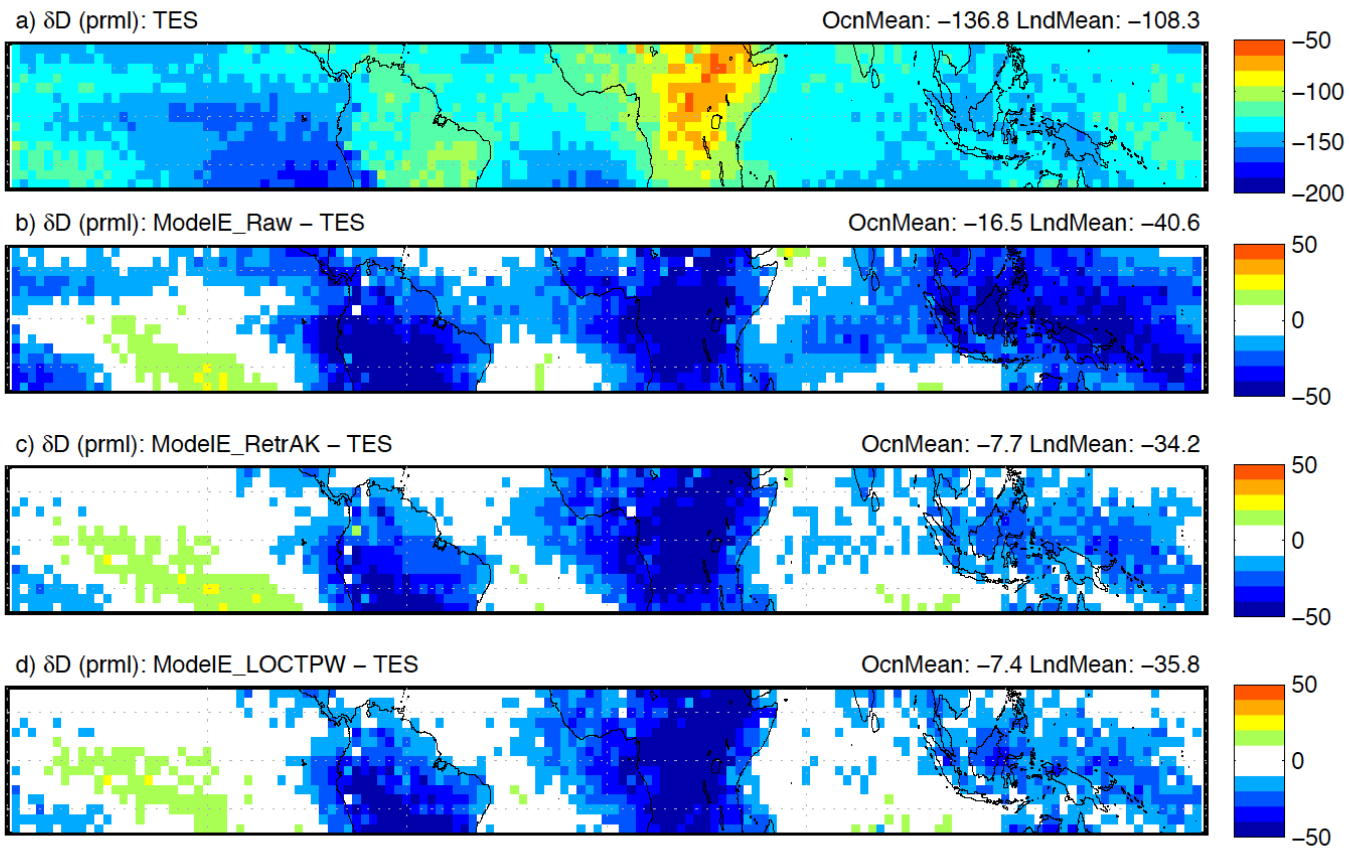
H_2O prior selection: also insensitive to selection of H_2O prior profile

Performance outside tropics

As implemented, poor.



TES vs. ModelE δD



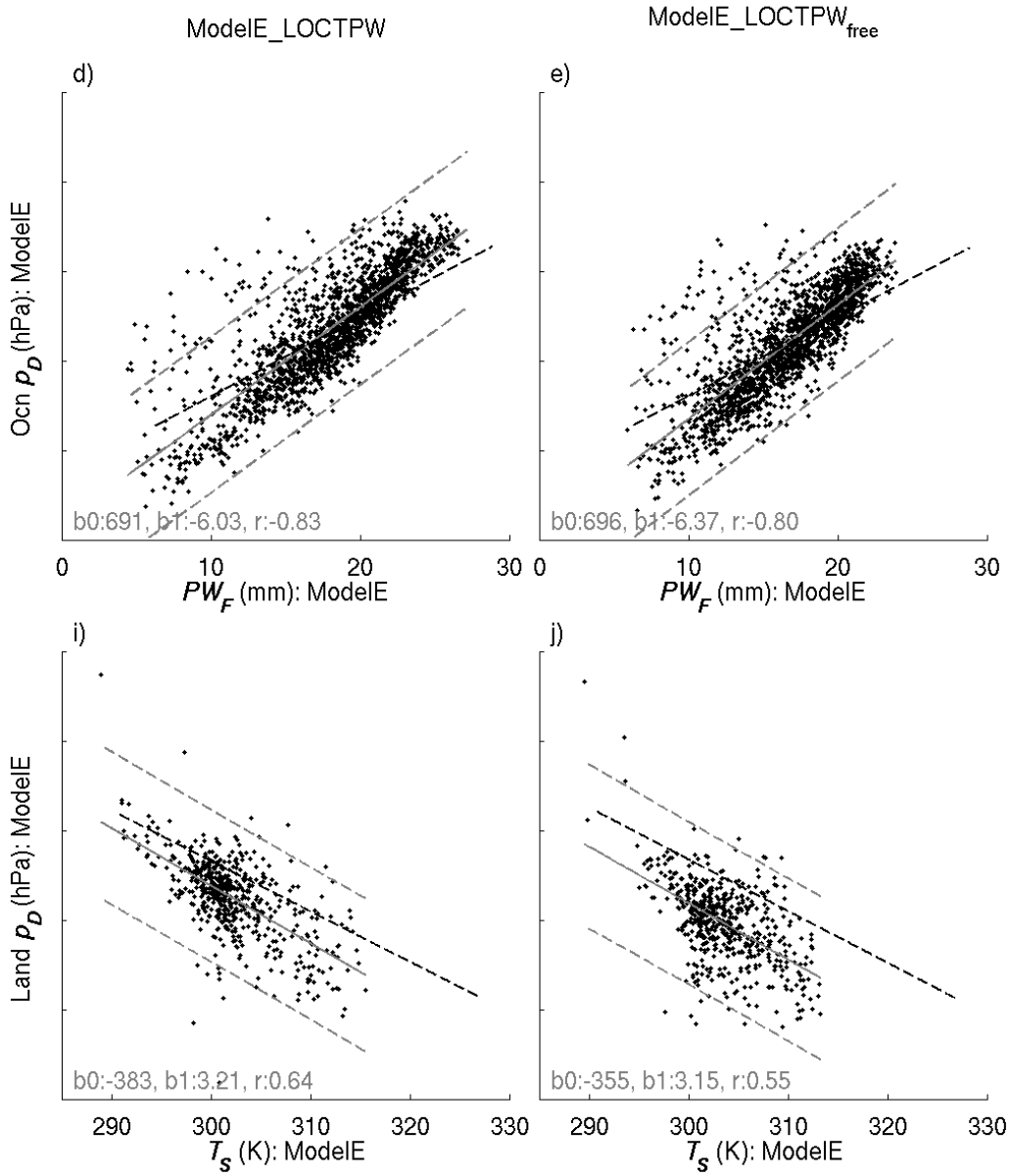
δD_{TES}

$\delta D_{Raw} - \delta D_{TES}$

$\delta D_{RetrAK} - \delta D_{TES}$

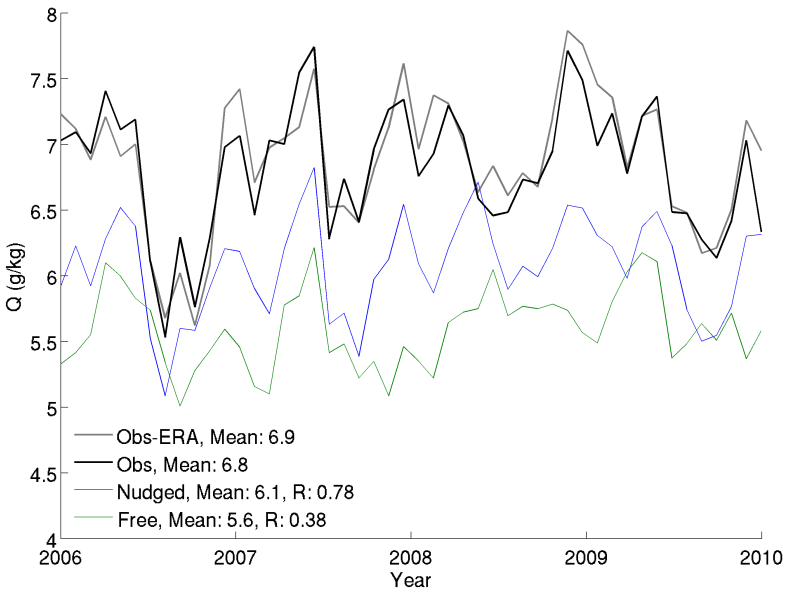
$\delta D_{CatAK} - \delta D_{TES}$

p_D controls for free running simulations

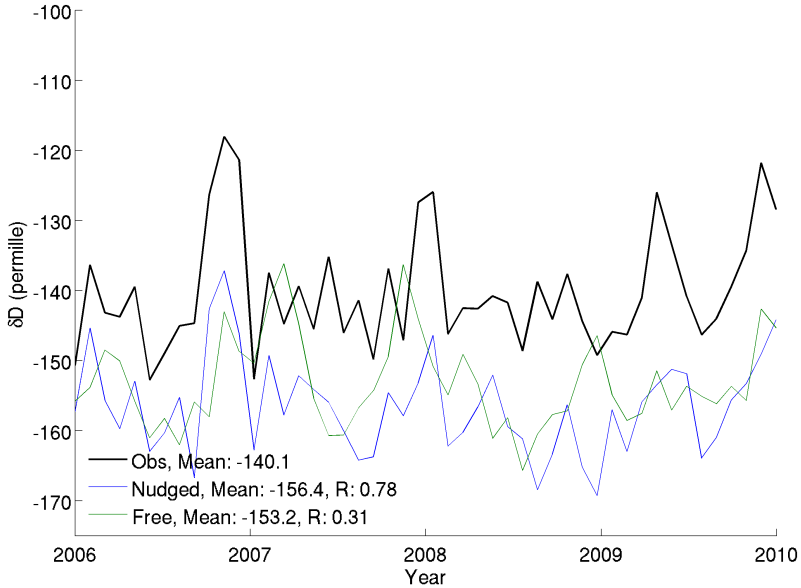


Interannual variability over Indonesia

Monthly Q



Monthly δD



Conclusions

- Cloud characteristics, surface temperature and free-tropospheric moisture were the most important predictors of retrieval quality and averaging kernel structure
- Application of the TES operator resulted in increases of up to 30 ‰ over the ocean and decreases of up to 40 ‰ over land
- Application of the TES operator significantly reduced the difference in δD between TES and ModelE
- The categorical operator can be used for arbitrary model configurations, and requires no agreement between satellite-retrieved and model meteorology at short time scales
- Refinements are needed for application outside of the tropics