
Chemistry Updates for CCMI

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11 February 2013

WACCM Working Group Meeting

NCAR

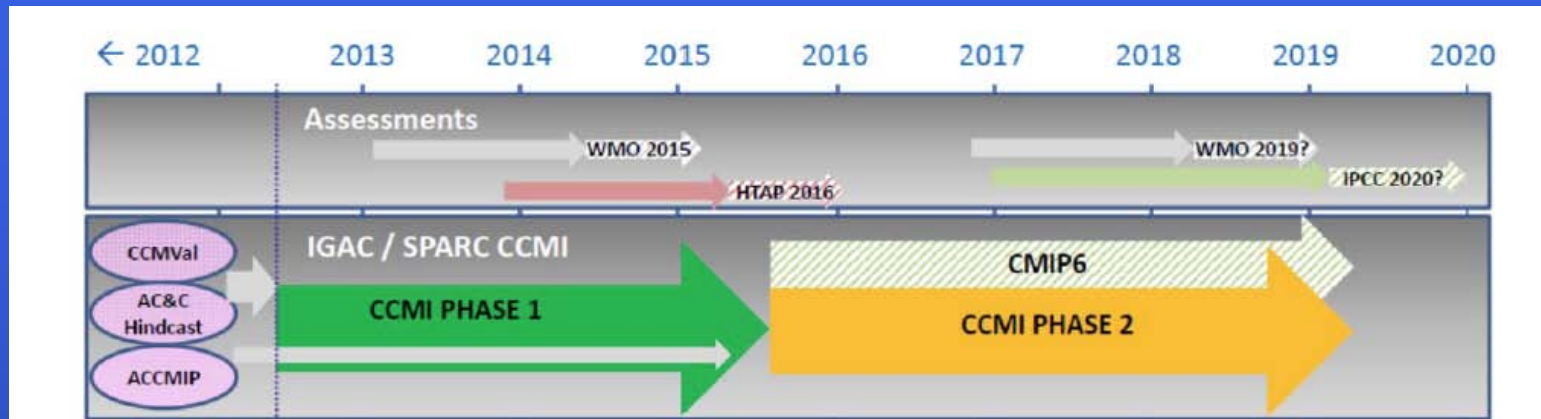
Why Do Another Assessment?

- **NESL / ACD community contribution.**
- **Increases national and international collaborations.**
- **Fosters model improvements (preparing for simulations).**
- **Creates new model diagnostics and model improvements after simulations are complete!**
- **Promotes scientific research.**

Recommendations from CCMVal2

- Inclusion of a more comprehensive representation of troposphere-stratospheric chemical processes. **DONE**
- Inclusion of VSL Organic Bromine species. **DONE**
- Inclusion of a couple ocean. **DONE**
- Inclusion of internally derived QBO. **Maybe**
- Correct the persistent late-spring breakdown of the Antarctic Vortex. **NO**
- Improve the representation of volcanic heating. **NO**

Chemistry Climate Model Initiative (CCMI)



- **First meeting was in May 2012 (Davos Switzerland).**
- Next meeting will be hosted by NCAR in May 2013.
- **The initial phase of CCMI will be to support the WMO 2015 O₃ Assessment.**
- Model simulation will start by 1 March 2013.
- **Model simulation will include "nudged" approaches for CCMI.**

Planned Simulations

Table 1. Summary of proposed IGAC/SPARC CCMi reference simulations.

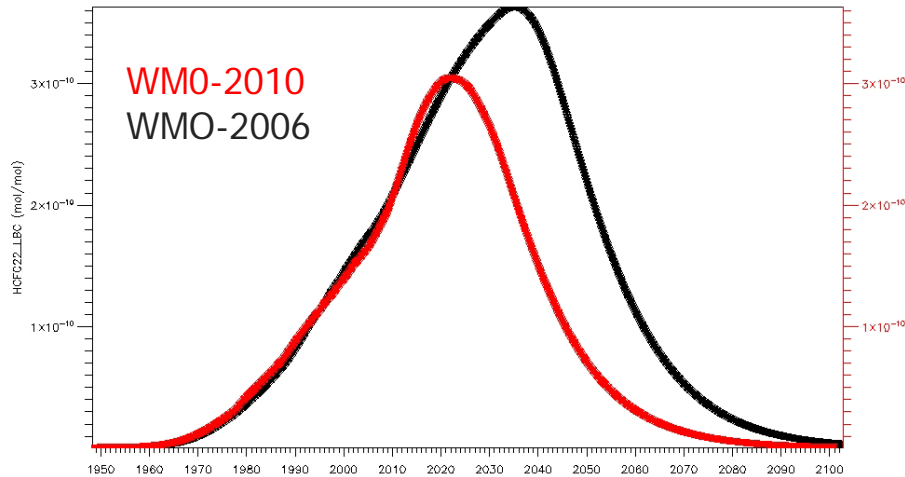
Name of Reference Simulation	Period	Greenhouse Gases	ODSs	SSTs/SICs	Background & Volcanic Aerosol	Solar Variability	VSLs	QBO	Ozone and Aerosol Precursors
REF-C1	Transient simulation 1960-2010 Appropriate spin up prior to 1960	OBS GHG used for CMIP5 simulations, updated until 2010.	OBS (WMO, 2011)	OBS HadISST1	OBS Surface Area Density data (SAD)	OBS Spectrally resolved irradiance data, Proton ionization, Ap	YES	OBS or internally generated	OBS Based on Lamarque et al. (2010), but annual emissions
REF-C1SD (nudged for CCMs, or CTMs)	Transient simulation 1980-2010	OBS Same as REF-C1	OBS Same as REF-C1	OBS Consistent with met. reanalysis	OBS Same as REF-C1	OBS Same as REF-C1	Same as REF-C1	Same as REF-C1	OBS Same as REF-C1
REF-C2	Transient simulation 1960-2100 10-year spin up prior to 1960	OBS to 2005 then RCP 6.0 (Masui et al., 2011)	OBS + A1 scenario from WMO (2011)	Modeled SSTs	OBS Background SAD	YES Spectrally resolved irradiance data, Proton ionization, Ap	YES	YES	Same as REF-C1 until 2000 + RCP 6.0 scenario in the future

Chemistry Updates

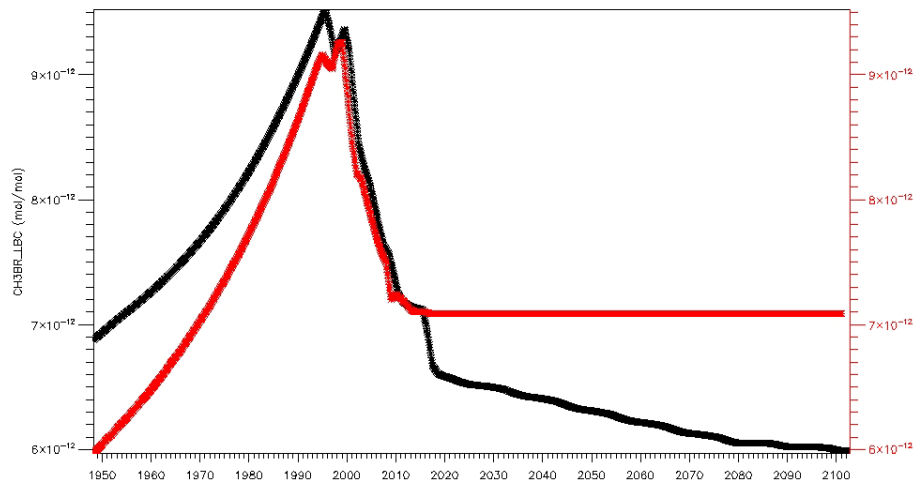
- **Organic Halogens**
- Tropospheric Chemistry Additions
- **Updated Heterogeneous Module**
- New Surface Area Density Time series
- **Rate and Satellite / Aircraft Output.**

Organic Halogens Updated to WMO-2010

HCFC -22



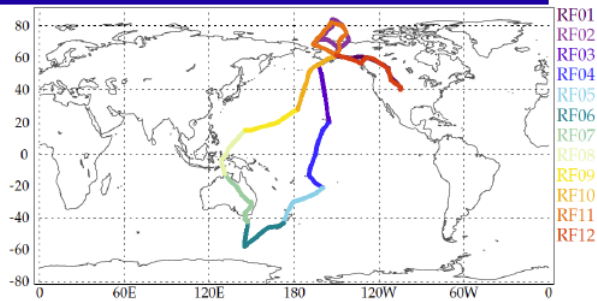
CH3Br



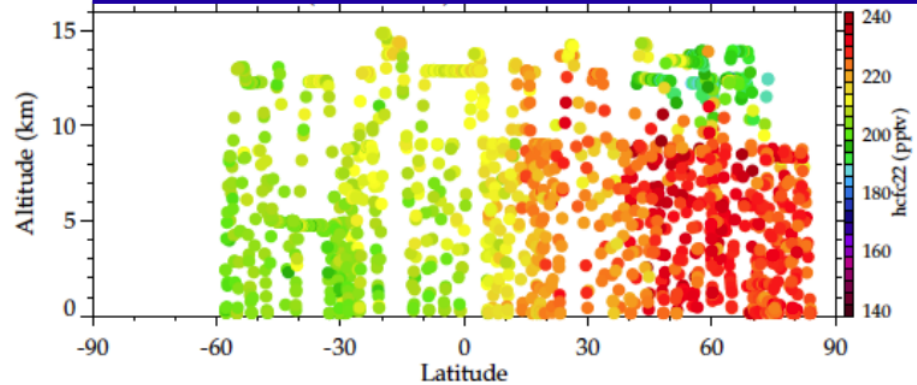
- **WMO-2010, Chapter 5**
 - SD-WACCM / MERRA
- **No Surrogates**
 - 18 species total
 - 8 new species
- **Long-lived (> 50 years)**
 - CFC-11, CFC-12, CFC-113, CFC-114, CFC-115, CCl₄, halon-1301
- **Medium (10-50 year)**
 - halon-1211, halon-1202, halon-2402, HCFC-22, HCFC-142b
- **Short (1-10 years)**
 - CH₃Cl, CH₃Br, CH₃CCl₃, HCFC-141b
- **Very Short Lived (<6months)**
 - CHBr₃, CH₂Br₂

Organic Halogens Latitudinal Gradient

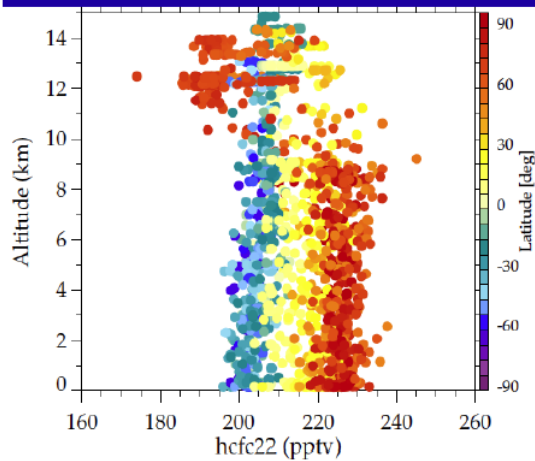
1. HIPPO-4 Flight Tracks (6/14-7/11, 2011)



2. HIPPO-4 HCFC22



3. HIPPO-4 HCFC22 profiles (color: latitude)



4. WACCM4 HCFC22 (interpolated to HIPPO-4)

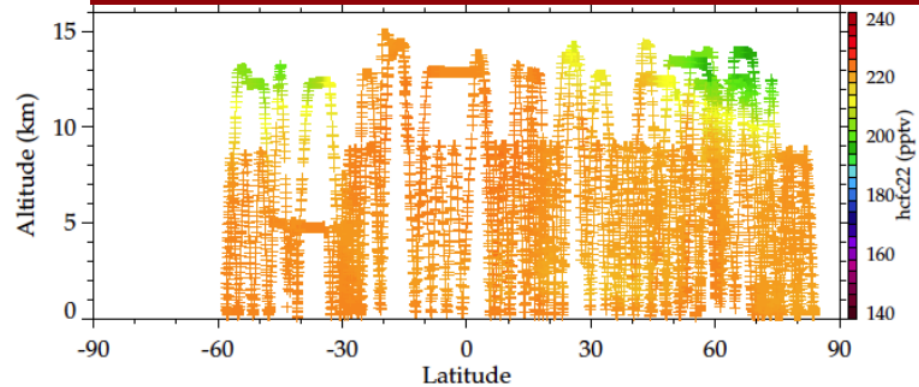
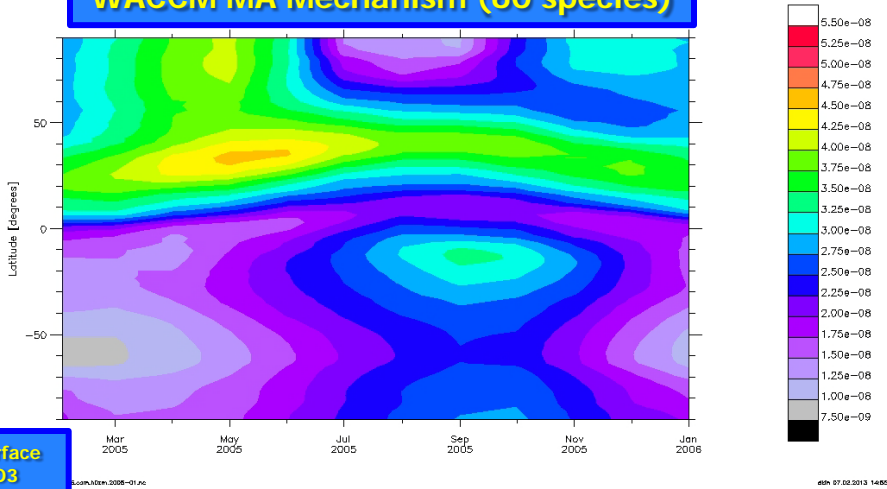


Figure Courtesy of M. Park

Inclusion of Tropospheric Chemistry (155 Species; 434 Rxns)

WACCM MA Mechanism (60 species)



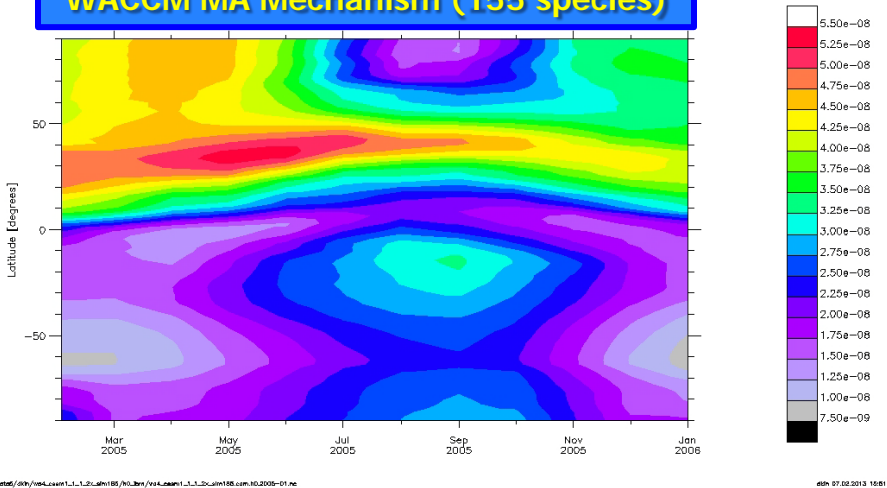
Standard Tropospheric Species

- CH₄, CO, CH₂O, CH₃COOH, CH₃O₂

Additional Tropospheric Species (srf emis)

- C1: CH₃OH, HCOOH, HOCH₂OO
- C2: C₂H₂, C₂H₆, C₂H₄, C₂H₅O₂, C₂H₅OH, C₂H₅OOH, CH₃CO₃, CH₃COOOH, EO₂, EO, EOOH, GLYALD, GLYOXAL, PAN
- C3: C₃H₆, C₃H₈, C₃H₇O₂, C₃H₇OOH, CH₃COCH₃, CH₃COCHO, PO₂, POOH, CH₃CHO, RO₂, ROOH, HYAC, ONIT
- C4: BIGENE, ENEO₂, MEK, MEKO₂, MEKOOH, MVK, MACR, MACRO₂, MACROOH, MCO₃, MPAN,
- C5: ISOP, ISOPO₂, ISOPNO₃, ISOPOOH, BIGALK, BIGALD, HYDRALD, ALKO₂, ALKOOH, ONITR, XO₂, XOOH
- C7: TOLUENE, CRESOL, TOLO₂, TOLOOH, XOH, TERPO₂, TERPOOH
- C10: C₁₀H₁₆
- Other: HCN, CH₃CN
- Aerosol: NH₃, OC1, OC2, CB1, CB2, DMS, SO₂.
- Emissions (CO, NO, NMHCs):
 - IPCC ACCMIP / CCMI (1950-2100).
 - Emmons (1992-2010)
- Bulk Aerosol Model (BAMS)
 - Sulfate, Black Carbon, Organic Carbon, and Ammonium Nitrate, SOA, SSLT(4), DST(4)

WACCM MA Mechanism (155 species)

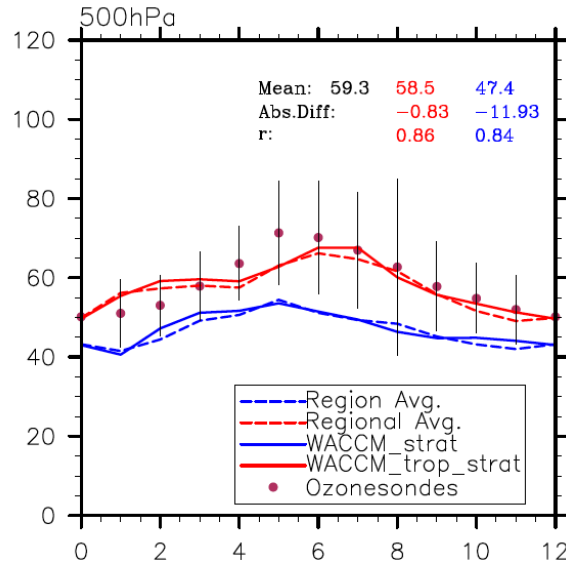
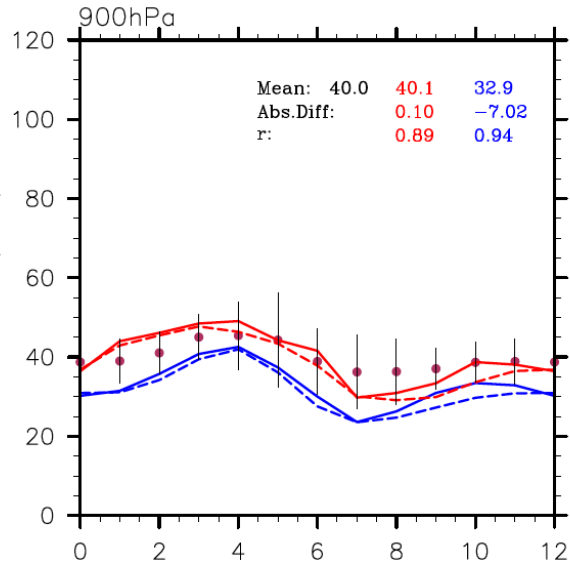


Acknowledge: G. Brasseur, J. F. Lamarque, L. Emmons, J. Orlando, C. Granier, et al.,

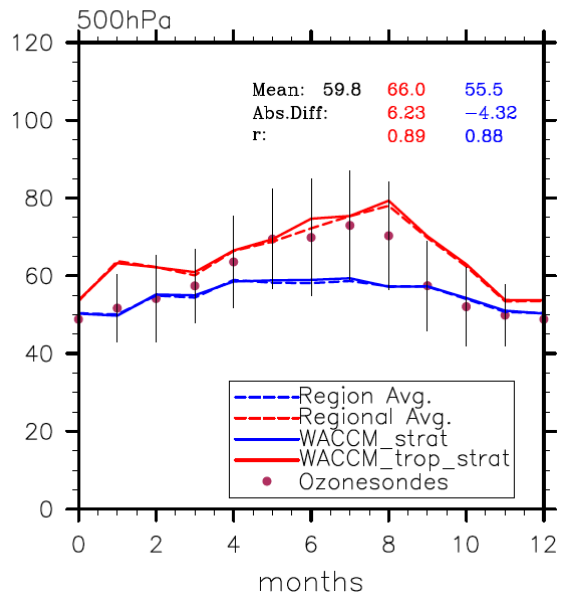
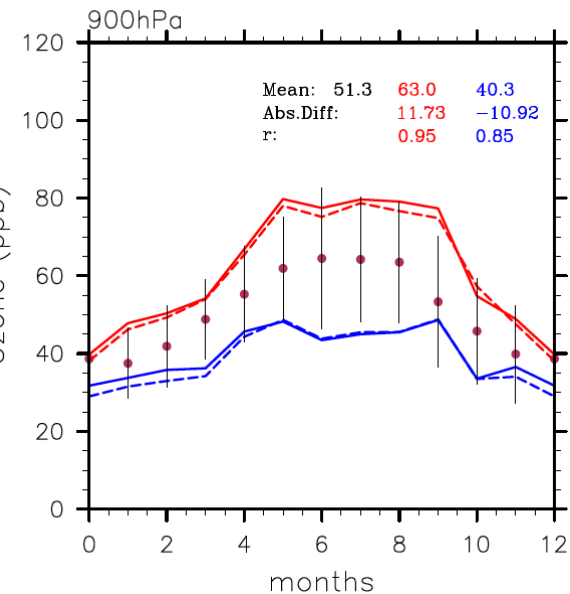
• Neu Wet deposition

Comparison to Ozone Sondes

NH Polar East



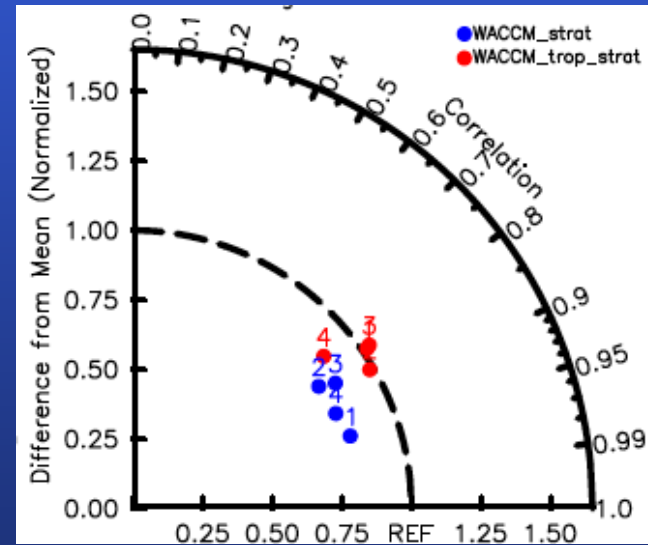
Eastern US



Ozonesondes

Strat/trop (155 species)

Strat. (60 species)



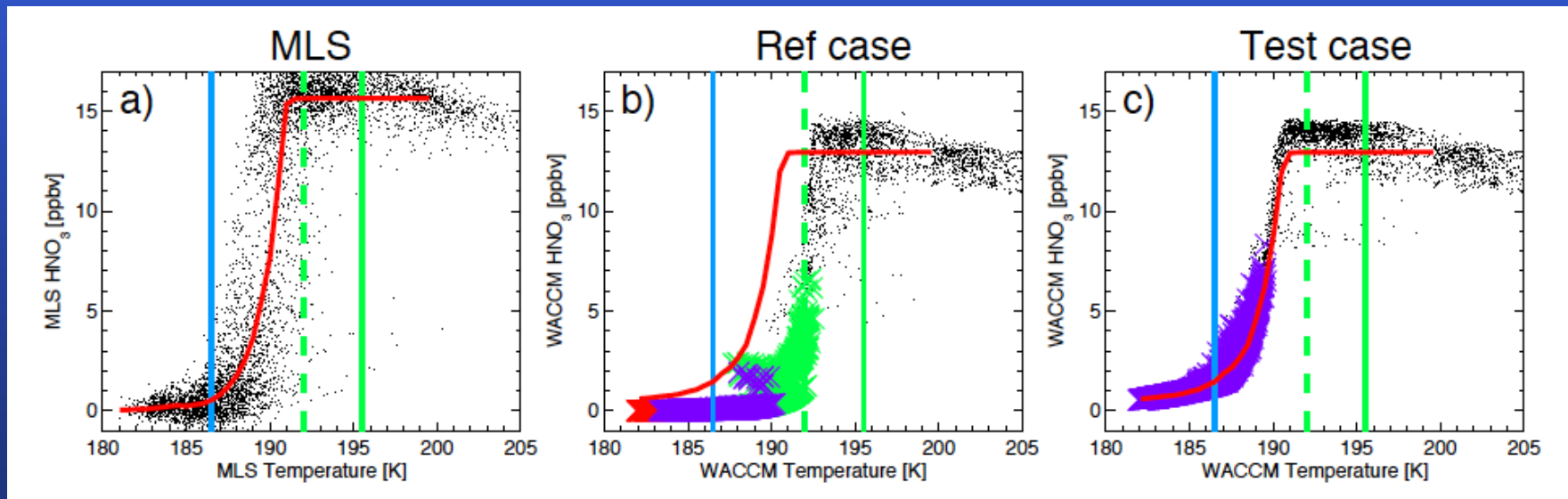
- 1: NH W Pol
- 2: NH E Pol
- 3: Canada
- 4: SH Polar

New Heterogeneous Module

Wegner, T, D. E. Kinnison, R. R. Garcia, S. Madronich, S. Solomon, and M. von Hobe, On the depletion of HCl in the Antarctic polar vortex, in review, *J. Geophys. Res.*, 2013.

Wegner, T, D. E. Kinnison, R. R. Garcia, S. Madronich, and S. Solomon, Polar Stratospheric Clouds in SD-WACCM4, in review, *J. Geophys. Res.*, 2013.

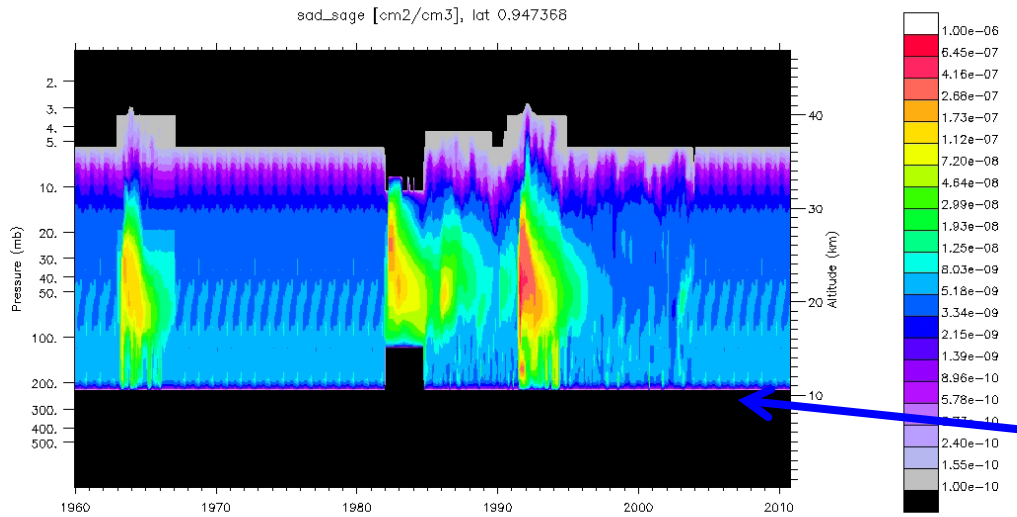
Brakebusch, M., C. E. Randel, D. Kinnison, S. Tilmes, M. Santee, and G. Manney, Evaluation of Whole Atmosphere Community Climate Model simulations of ozone during Arctic winter 2004-2005, *in press*, *J. Geophys. Res.*, 2012.



Also improved the representation of dehydration.

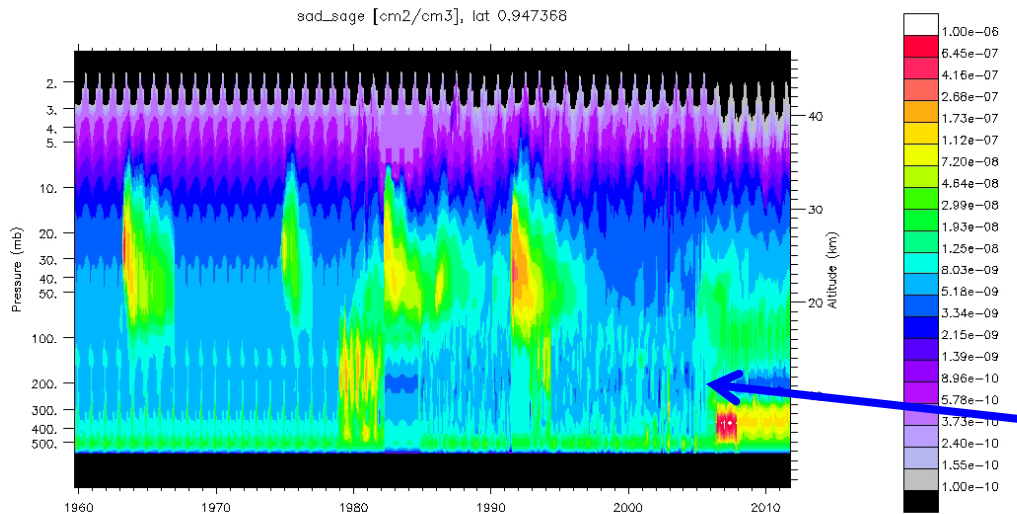
Set a rhminh for the stratosphere (dehydration starts at 100% saturation of H₂O over ICE).

New Sulfate Surface Area Density Time Series



CCMVal-2 SAD

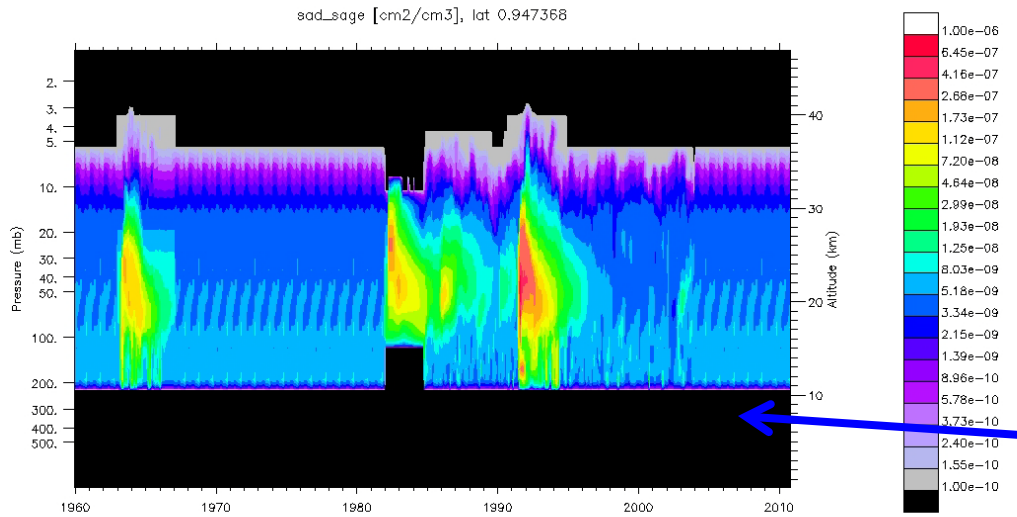
SAD zero for P > 200 hPa



CCMI SAD

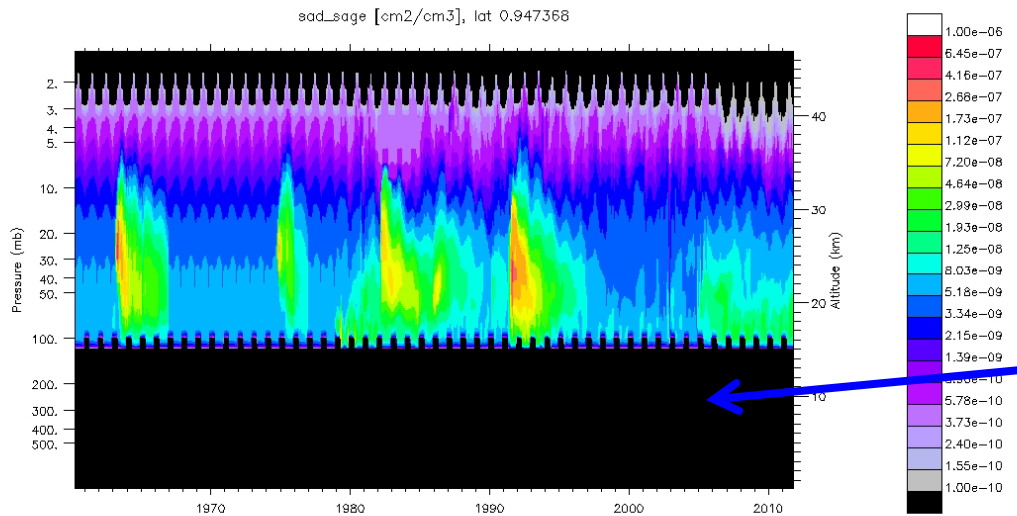
Note the volcanic influence below the tropopause.

New Sulfate Surface Area Density Time Series



CCMVal-2 SAD

SAD zero for P > 200 hPa



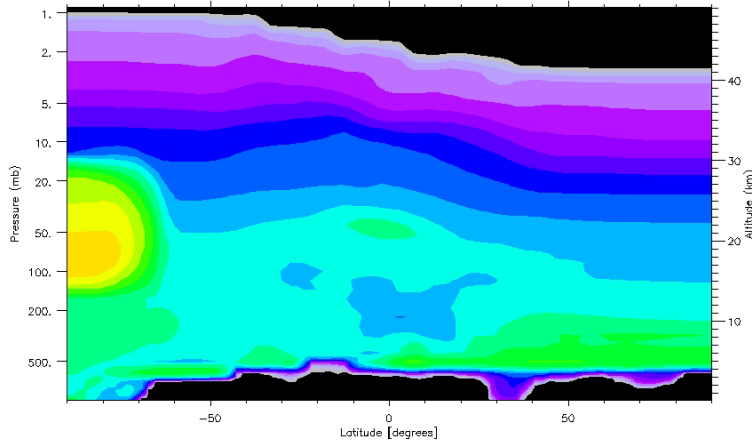
CCMI SAD

Zero SAD below Tropopause.

Ryan Neeley is currently examining impact of SAD time series.

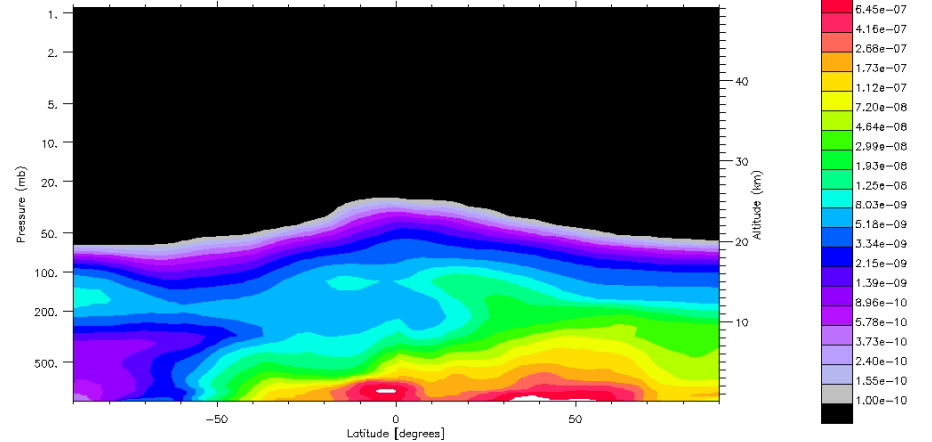
Stratospheric and Tropospheric SAD (BAMS) - July

Stratospheric SAD



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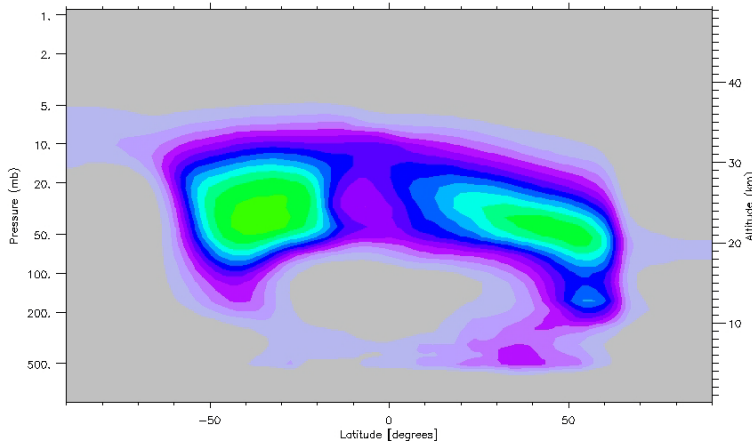
BAMS SAD



/home/ghy/vel/eam1.1.2/eam179/10/vel/eam1.1.2/eam179/eam10.2008-07.nc

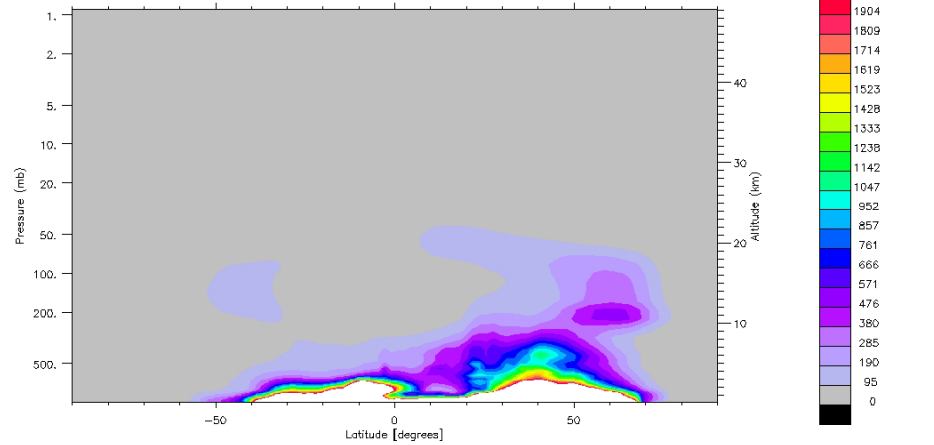
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Stratosphere N₂O₅ + H₂O Rate



/home/ghy/vel/eam1.1.2/eam179/10/vel/eam1.1.2/eam179/eam10.2008-07.nc

BAMS N₂O₅ + H₂O Rate

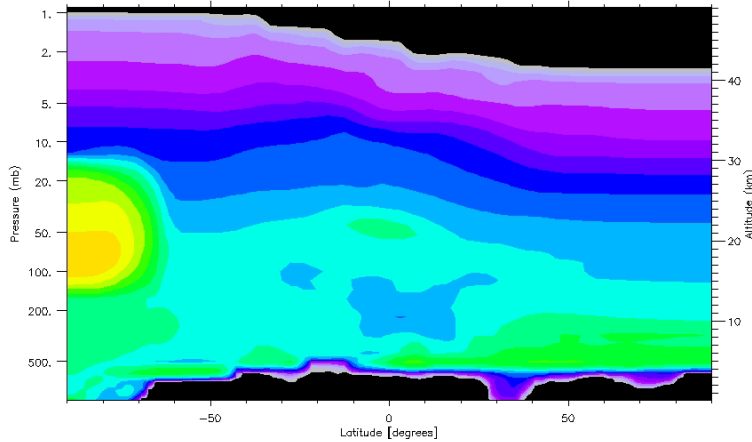


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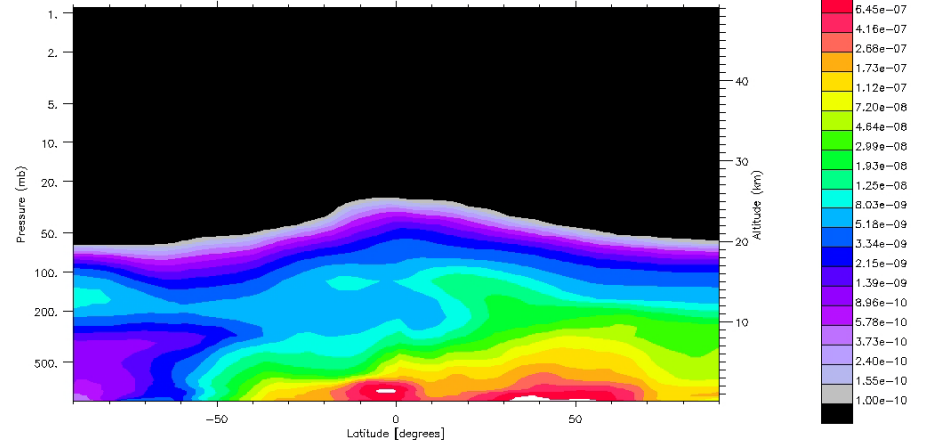
Stratospheric and Tropospheric SAD (BAMS) - July

Stratospheric SAD



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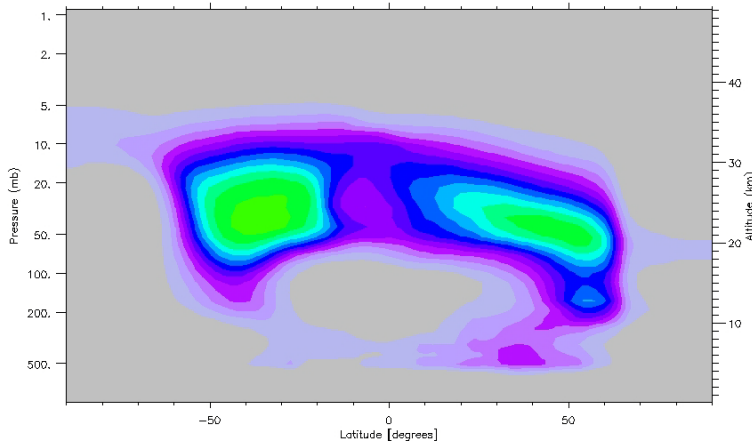
BAMS SAD



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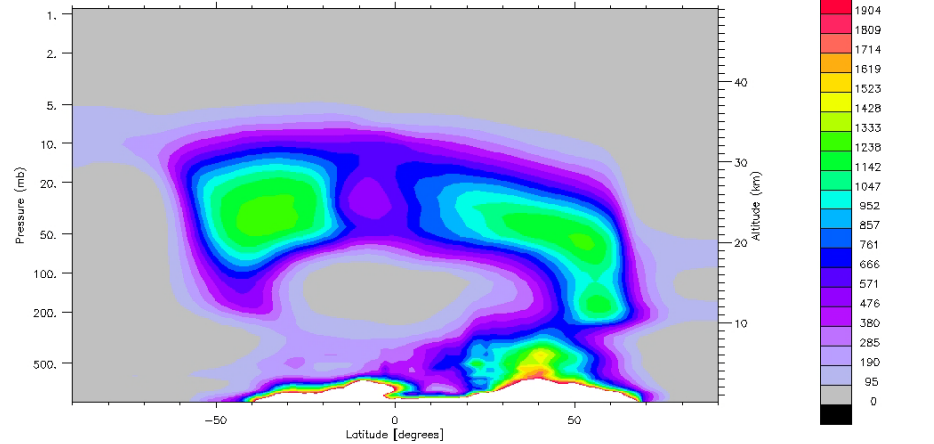
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Stratosphere $N_2O_5 + H_2O$ Rate



/media/ghcn/v6/Leam1.1.20.am179/10/v6/Leam1.1.20.am175.am10.2008-01.nc

Total $N_2O_5 + H_2O$ Rate



/media/ghcn/v6/Leam1.1.20.am179/10/v6/Leam1.1.20.am175.am10.2008-01.nc

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Volcanic Heating

Procedure to derive heating rates:

- 1) Derive Volume Density (cm^{-3} aer / cm^3 air)
 - Function (SAD, size distribution, # particles)
- 1) Density of H_2SO_4 Aerosol ($\text{g aer} / \text{cm}^3$ aer)
 - Liquid binary model (Tabazedeh, 1997)
- 1) Weight fraction ($\text{g H}_2\text{SO}_4 / \text{g Aer}$)
 - Tabazedeh et al., 1997.

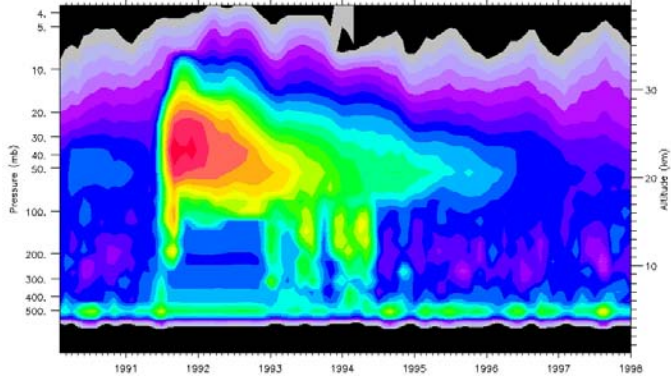
Chemistry: $\text{g H}_2\text{SO}_4 \text{ cm}^{-3}$ air

Radiation wants: H_2SO_4 in kg m^{-2}

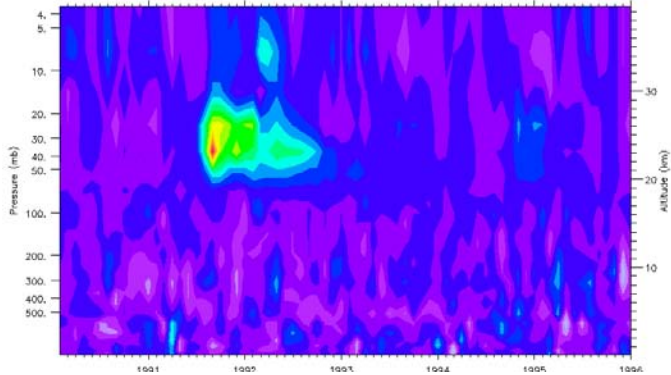
CAMRT Derives Heating

- Optics: 75% wt; 0.5 micron

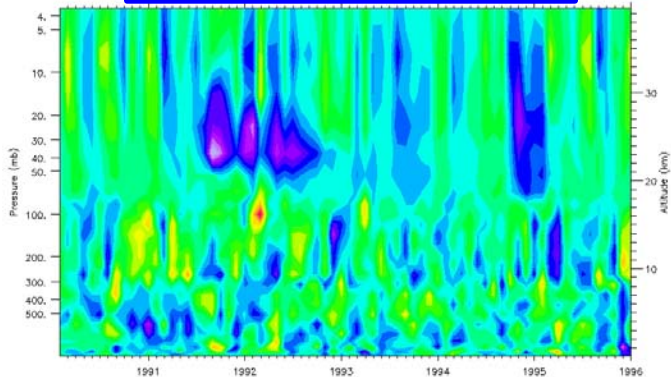
SAD $\text{cm}^2 \text{cm}^{-3}$ *** Tropics



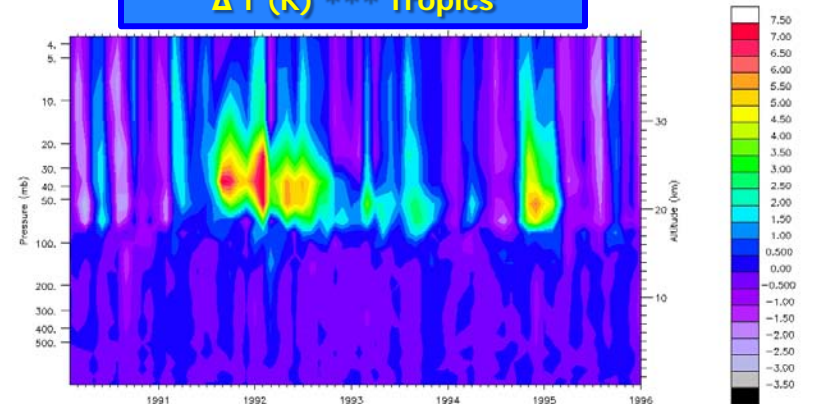
Δ QRS (K sec^{-1}) *** Tropics



Δ QRL (K sec^{-1}) *** Tropics



Δ T (K) *** Tropics



Satellite Output for SD Simulation.

Don't have =>

Don't have =>

	O ₃	H ₂ O	CH ₄	N ₂ O	CCl ₃ F	CCl ₂ F ₂	CO	HF	SF ₆	NO	NO ₂	NO _x	HNO ₃	HNO ₄	N ₂ O ₅	ClONO ₂	NO _y	HCl	ClO	HOCl	BrO	OH	HO ₂	CH ₂ O	CH ₃ CN	aerosol
ACE-FTS	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x							x	
Aura-MLS	x	x		x			x						x					x	x	x		x	x			
GOMOS	x										x															x
HALOE	x	x	x					x		x	x	x						x								
HIRDLS	x				x	x					x		x													
LIMS	x	x									x		x													
MAESTRO	x																									
MIPAS	x	x	x	x	x	x	x		x	x	x	x	x	x	x	x	x		x	x				x		
OSIRIS	x										x	x _d					x _m				x					x
POAM II	x										x															x
POAM III	x	x									x															x
SAGE I	x																									
SAGE II	x	x									x															x
SAGE III	x	x									x															x
SCIAMACHY	x	x									x	x _d										x				x
SMILES	x												x					x	x	x	x		x		x	
Odin/SMR	x	x		x			x			x			x					x _m		x				x		
TES	x						x																			
UARS-MLS	x	x											x							x						

In additions:

- BUV, SBUV Nimbus 7,9,11,14,16,17,18,19
- CONCORDIASI PSC (6-balloon campaign)
- SOFIE
- SABER
- PEX 2005, 2010
- RECONCILE 2010
- SME

Acknowledge: Matthias Brakebusch (CU) for assembling coordinate file.

Aircraft Output

TBD!



Thank you for your attention!