Chemical Forecasts and Field Modeling

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Rafael Fernandez-Cullen, Tom Hanisco, Neil Harris,
Cameron Homeyer, Shawn Honomichl, Doug Kinnison,
Jean-Francois Lamarque, Qing Liang, Julie Nicely,
Laura Pan, Alfonso Saiz-Lopez, Simone Tilmes, Glenn Wolfe
and many others ☺

23 Oct 2013

CONTRAST

Guam, Jan–Feb 2014

Source: Doug Kinnison

NCAR CESM CAM-CHEM

- Global Chemistry-Climate Model
- 1.9° (lat) x 2.5° (lon) horizontal resolution
- 26 vertical levels (surface to ~ 4 hPa)

Lamarque et al., *Geosci. Mod. Dev.*, 2012

Tropospheric Halogen Chemistry

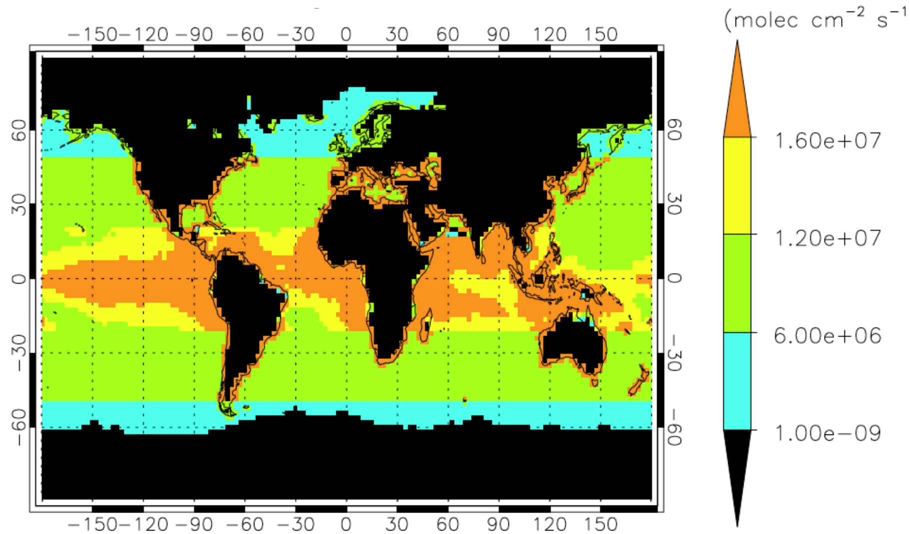
Halogenated sources from the ocean.

- Emissions following Chl-a over tropics
- Catalytic release from sea-salt
- Do NOT have polar emission processes

Chemical Processes

- Photochemistry (Cl, Br, and I)
- Dry / wet deposition
- 9 Additional vsl Organic species included.
- 160 species, 427 reactions

$CHBr_3$ Flux in CAM-Chem



Source gas	Global annual flux ($Gg\ yr^{-1}$)		Lifetime (this study)
	This study	Literature	
$CHBr_3$	533	400[a], 595[b], 448[d]	17 days
CH_2Br_2	67.3	113[c], 62[d]	130 days
CH_2BrCl	10.0	6.8[c]	145 days
$CHBr_2Cl$	19.7	23[c]	56 days
$CHBrCl_2$	22.6	16[c]	46 days
CH_3Br*	climatology	131[c]	1.6 yr[g]
CH_3I**	303	304[e]	5 days
CH_2ICl	234	236[f]	8 h
CH_2IBr	87.3	87[f]	2.5 h
CH_2I_2	116	116[f]	7 min

Total Bromine: 632 Gg Br yr^{-1}

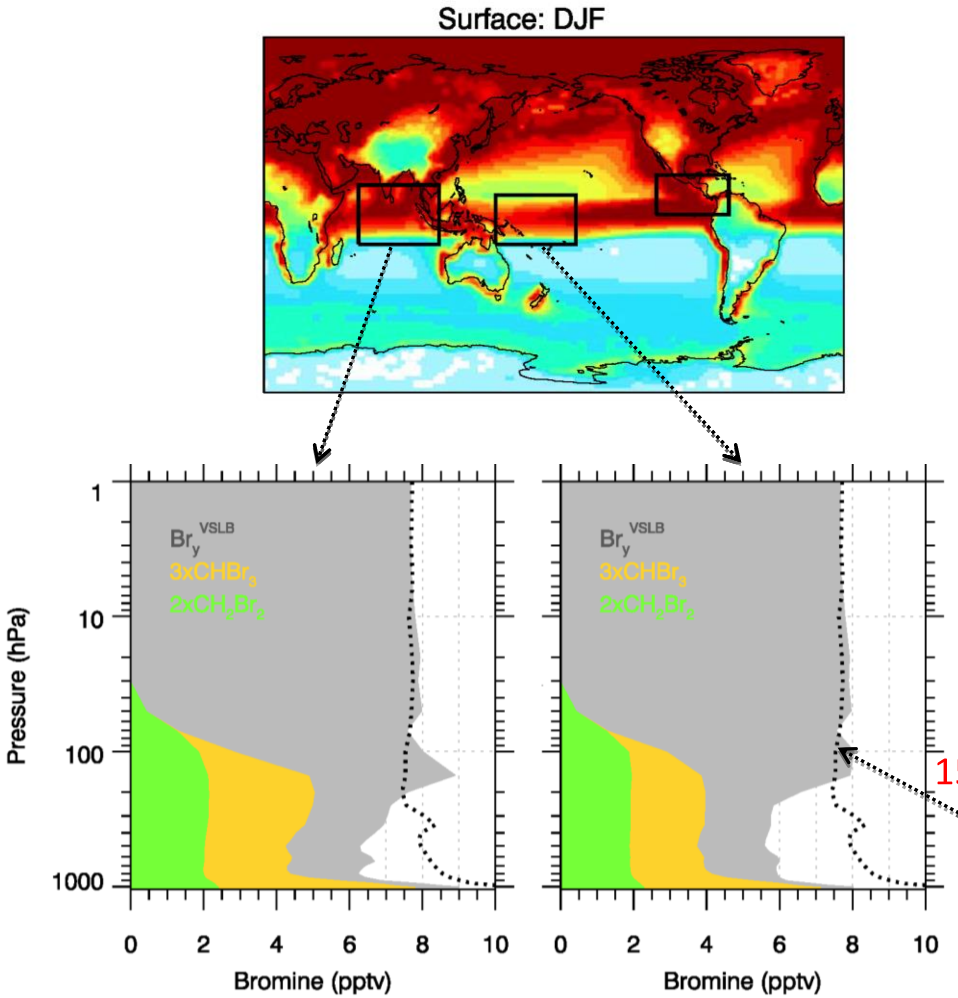
Total Iodine: 600 Gg I yr^{-1}

Ordoñez et al., ACP, 2012

Source: Qing Liang

Prior obs & modeling: SGI (source gas injection) of Br_y is probably 5 to 7 ppt

Prior obs & modeling: PGI (product gas injection) of Br_y highly uncertain: depends on efficiency of aerosol uptake and washout versus het chem release of labile bromine and strength of convection (Q. Liang talk)



150hPa(355K)

Super efficient convective lofting: The mixing ratio of total bromine from VSLB (organic + inorganic) at 150 hPa (~355K) is about 8.0 - 8.5 ppt, similar to the surface abundance.

Global Mean Br_y^{VSLB} ~ 7.7 ppt throughout stratosphere.

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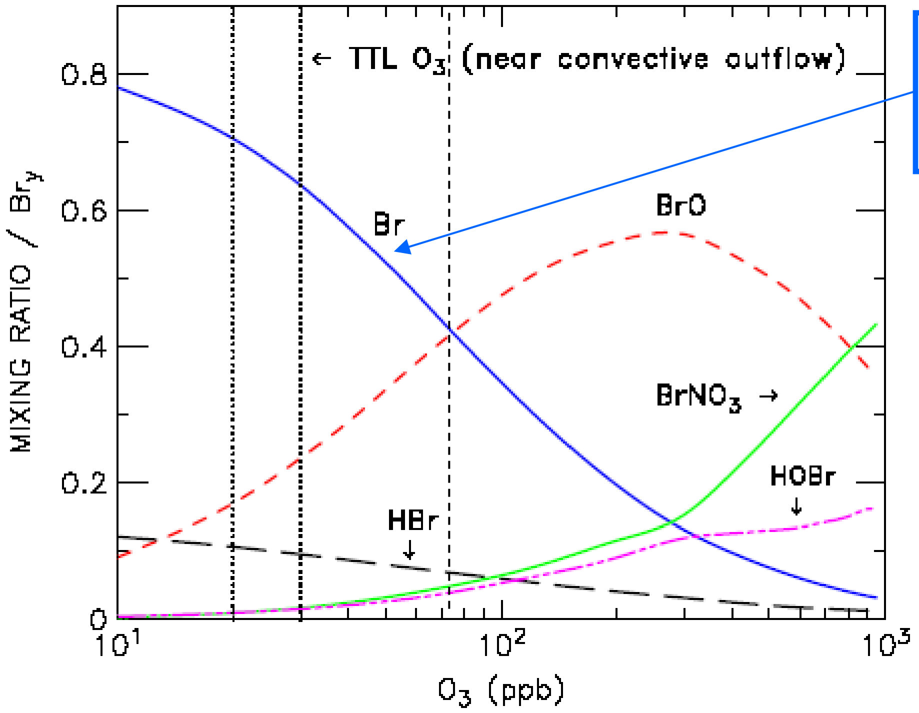
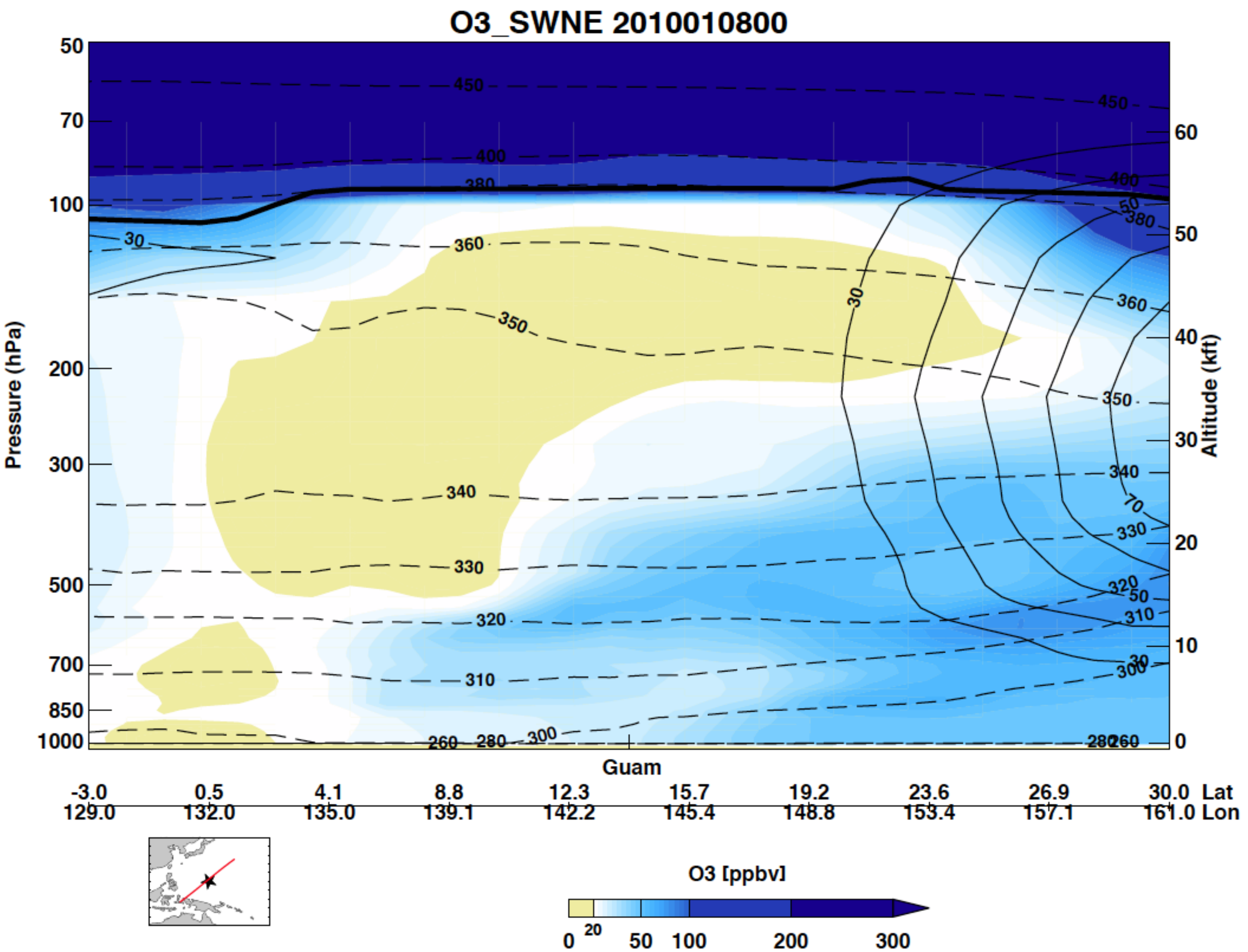


Br + HCHO is believed to be the primary route out of Br-reservoir for low O_3 conditions

Source: Doug Kinnison & Laura Pan

Example SW-NE cross section from SD-WACCM



Chemical Forecast Plan:

- NCAR CESM CAM-CHEM forecast simulations to occur in Boulder
- 3 day forecasts will be available every ~24 hrs using GEOS5 met fields
- forecasting will begin with ferry flights
- domain-wide plots to be generated via script
- curtain plots along candidate flight trajectories possible: probably implemented by folks in Guam providing ASCII file with flight coordinates to server in Boulder, with plots generated in Boulder
- at this time we are not planning to transfer model files to Guam
- besides O_3, we intend to examine fields of:
  - H_2O, CH_4, CO
  - 10 VSLs listed on slide 5 plus a few select ratios
  - OH, HO_2, HCHO, NO, NO_2, BrO, Br/BrO, IO (daytime active species)
  - HBr, HOBr, $BrNO_3$, BrCl (dawn/dusk flights)

A chemical modeler’s / co-mission scientist wish list ☺

Class 1	**O_3**
Class 2	**CO, H_2O & CH_4** **CH_2Br_2, $CHBr_3$, CH_3I, etc** **NO_x, OH, HO_2, HCHO**
Class 3	**BrO, BrO/Br_y, IO : daytime flights** **HBr, HOBr, $BrNO_3$, BrCl : dawn/dusk flights** **Non-methane precursors of HO_x & HCHO (H_2O_2, acetone, isoprene, ethane, etc)**

Class 1 ⇨ as many vetted models as possible
Class 2 ⇨ multiple models very helpful
Class 3 ⇨ at least one model

Near Real Time TOMCAT/SLIMCAT Model Simulations

Hannah Mantle, Ryan Hossaini, Martyn Chipperfield

University of Leeds, UK

- Forced by ECMWF operational analyses. Available within 1 day of analysis time.
- Model resolution up to e.g. 1^o x 1^o.
- Run could include 'full ' chemistry (stratosphere/troposphere).
- Can include tracers for different emission fields (e.g. 4 different $CHBr_3$ emission datasets).
- Can provide sample at stations and along flight tracks for 'first look' comparisons.

Can set up web page. See example from SHIVA campaign:
www.see.leeds.ac.uk/slimcat
http://homepages.see.leeds.ac.uk/~earrh/SHIVA_SITE/

Other possible sources of forecast information:

MACC: Monitoring atmospheric composition and climate

http://www.gmes-atmosphere.eu

Standard products: O_3, CO, NO_x, HCHO, and SO_2

Surface, 850, 500, 300, and 30 hPa

Field campaign support available upon request

http://www.gmes-atmosphere.eu/services/aqac/campaign_support

D-AQ: Total AOD, Dust, Sea-Salt, Sulphate, Black Carbon, Organic Matter

TRAQA: Dust, Black Carbon, tagged CO (South Asia, W. Europe, E. Europe N. Africa, Europe Biomass-burning)

MOZART−4 MOPITT

http://www.acd.ucar.edu/acresp/forecast

Standard products: O_3, CO, tagged CO, NO_x, and PAN

Surface, 4 km, 10 km, and column

CO tags: fires, NA, Europe, India, E. Asia

Output routinely provided on line

Tool developed for air pollution applications; the higher in altitude the more the product is influenced by climatology

Other possible sources of forecast information:

RAQMS: Real Time Air Quality Modeling System

http://raqms-ops.ssec.wisc.edu

Standard products: O_3, CO, H2O, DMS, HCHO, Aerosol Extinction
Surface, 3, 6, and 12 km

5 day 1x1 degree global forecasts

Will archive:

- **transported stratospheric & tropospheric chemical species, radicals (OH, BrO, NO, NO_2, etc..) and speciated (GOCART) aerosol wet/dry mass and extinction.**
- **dynamical quantities (u,v,t,z,p,pv) &**
- **physics (convective cloud mass flux, cloud optical depth, large-scale and convective precip).**

Box Modeling Plan:

- Julie & Tim will be conducting box model simulations along the GV flight track in the field, with a focus on OH
- Glen & Dan will also be conducting box model simulations along the GV track in the field, with a focus on HCHO
- box modeling by others encouraged, either during or after deployment !
- box modeling requires a suite of GV measurements as inputs
- in my prior life as stratospheric modeler, we could used tracer/tracer relations to fill in gaps until data became available
- data gaps not easily filled in the tropical troposphere: *modelers must clearly communicate to instrument team which observations are needed as input to various box models*

Initial list: O_3, H_2O, CH_4, CO, NO, NO_2, C_2H_6, C_3H_8, C_5H_8, C_2H_2O, C_3H_6O, J_{O1D}, J_{NO2}, Aerosol Surface Area

NRT access to $CHBr_3$, CH_2Br_2, and CH_3I also very important