



# Validation Protocol: Nadir Ozone Profile Update

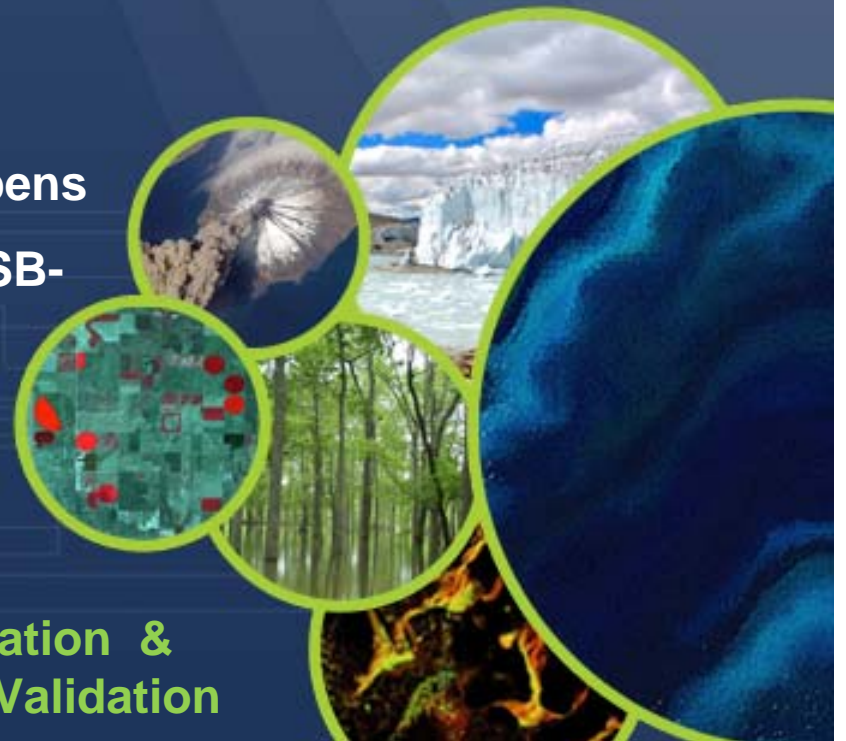
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BIRA)

ACC Meeting #11

ESA/ESRIN, Frascati, Italy

April 28 - 30, 2015

CEOS Atmospheric Composition Constellation &  
CEOS Working Group on Calibration and Validation



## Total Ozone Validation Protocol

### Atmospheric Composition Constellation Meeting (ACC-9)

18-19 April 2013, EUMETSAT

#### I. Introduction

The next CEOS ACC meeting will take place on April 18-19 2013 at EUMETSAT ([www.eumetsat.int](http://www.eumetsat.int)) with a duration of 2 full days. During the first day we will have a total ozone workshop on recent algorithm upgrades, ancillary data used (cross sections, climatologies), geophysical validation and inter-comparison of the latest long term total ozone column data sets as produced in the USA and in Europe. In order to harmonise validation work to be done in preparation of the meeting, it has been agreed that a validation protocol will be defined, as follows.

The purpose of the validation protocol is to define a restricted set of common validation parameters and analyses. In this way, results obtained by different validation groups using different references data sets can be better compared and discussed.

#### II. Validation protocol



#	Harmonisation point	Description/ comments
1	Use same formula for relative difference	100*[Satellite - Ground]/Ground
2	Use same co-location criteria for Dobson and Brewer	Brewer and Dobson comparisons use daily mean WOUDC datasets. For each common day of measurements, the closest satellite measurement to the ground latitude sunrise-sunset satellite measurement.
3	Use same data filtering criteria	For <b>SBUV</b> : For <b>TOMS</b> :
5	Use same statistical estimators	

$$\text{Mean} = \bar{x} = \frac{1}{N} \sum_{j=0}^{N-1} x_j$$

$$\text{Variance} = \frac{1}{N-1} \sum_{j=0}^{N-1} (x_j - \bar{x})^2$$

$$\text{Standard Deviation} = \sqrt{\text{Variance}}$$

**SAZ bins:** from 0 to 90 degrees in steps of integral 5 degrees, i.e. from 0 to 5, from 5 to 10, etc.

**LAT bins:** from -90 to 90 degrees in steps of integral 10 degrees, i.e. from -90 to -80, from -80 to -70, etc.

**CTP bins:** from 50 to 1050 mbars in steps of 50 mbars, i.e. from 50 to 100, from 100 to 150, etc.

**CF bins:** from 0 to 1 in steps of 0.1, i.e. from 0.1 to 0.2, from 0.2 to 0.3, etc.

**O3VCD bins:** from 100 to 550 DU in step of 25 DU, i.e. from 100 to 125, from 125 to 150, etc.

**Effective-T° bins:** from 210 to 240 K in steps of 2° K

Note: It is recommended to filter the value if the RD is larger than the mean + or - 3 sigma.

8	Set of common plots (MRD = mean relative difference)	<ul style="list-style-type: none"> <li>- Monthly MRD vs time (NH, SH),</li> <li>- Daily MRD vs. SAZ,</li> <li>- Daily MRD vs. CF,</li> <li>- Daily MRD vs. CTP,</li> <li>- Daily MRD vs. O3VCD,</li> <li>- Daily MRD vs. lat,</li> <li>- Daily MRD vs. T°</li> <li>- Monthly MRD vs. Month of Year [=Jan to Dec]</li> </ul> <p>Unless otherwise stated, the above analysis should be performed on a global scale</p>
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### III. List of selected high-quality ground-based stations

#### 1. Dobson and Brewer stations from WMO/WOUDC

Station Name	Station Latitude	Station Longitude	WMO station number
Amundsen-Scott, Antarctica	-89.98	-24.8	111
Arosa, Switzerland	46.77	9.67	35
Arrival Heights, Antarctica	-77.83	166.4	268
Aswan, Egypt	23.58	32.27	245
Barrow, USA	71.32	-156.6	199
Belsk, Poland	51.50	20.47	68
Bismark, N.D., USA	46.77	-100.75	19
Boulder, CO, USA	40.02	-105.25	67
Brisbane, Australia	-27.47	153.03	27
Bucharest, Romania	44.48	26.13	226
Buenos-Aires, Argentina	-34.58	-58.48	91
Cairo, Egypt	30.08	31.28	152
Caribou, ME, USA	46.87	-68.02	20
Casablanca, Morocco	33.57	-7.67	158
Chengkung, Taiwan	23.1	121.36	306
Churchill, Canada	58.55	-94.07	77
Comodoro Rivadavia, Argentina	-45.78	-67.5	342
Dunedin, Australia	43.47	150.83	84

# QA / Validation Process

## for Nadir Ozone Profile Retrievals

Atmos. Meas. Tech. Discuss., 7, 11481–11546, 2014  
[www.atmos-meas-tech-discuss.net/7/11481/2014/](http://www.atmos-meas-tech-discuss.net/7/11481/2014/)  
 doi:10.5194/amtd-7-11481-2014  
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Atmospheric  
Measurement  
Techniques  
Discussions



This discussion paper is/has been under review for the journal Atmospheric Measurement Techniques (AMT). Please refer to the corresponding final paper in AMT if available.

## Round-robin evaluation of nadir ozone profile retrievals: methodology and application to MetOp-A GOME-2

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Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper

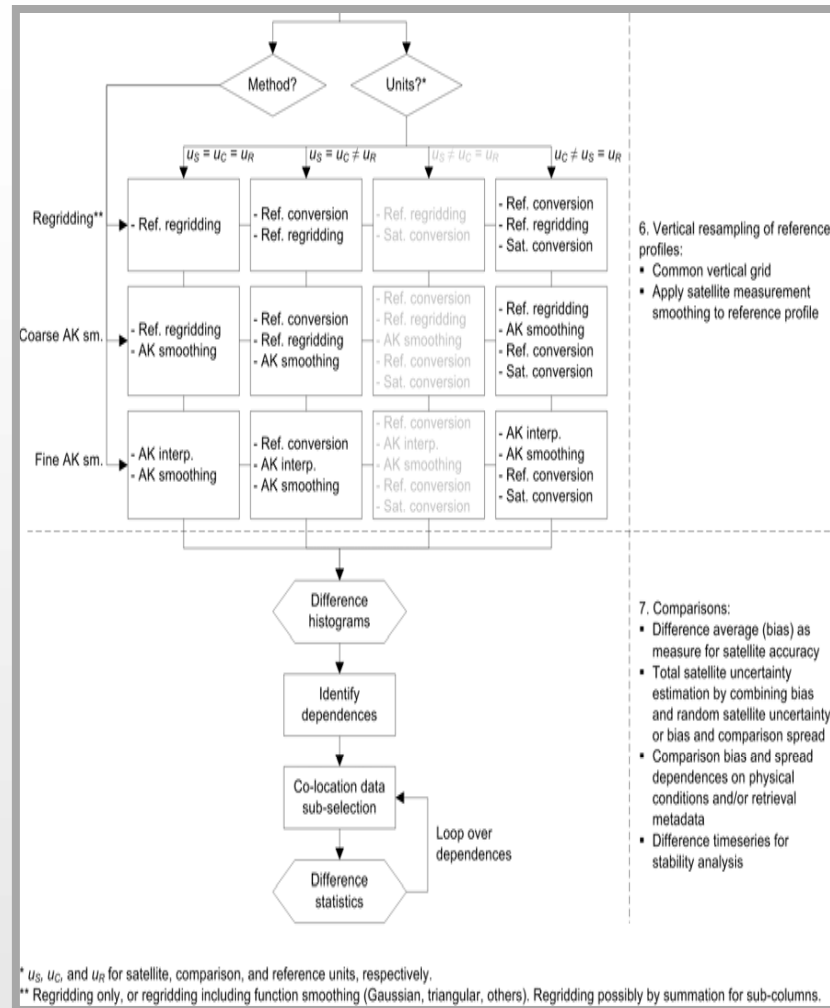
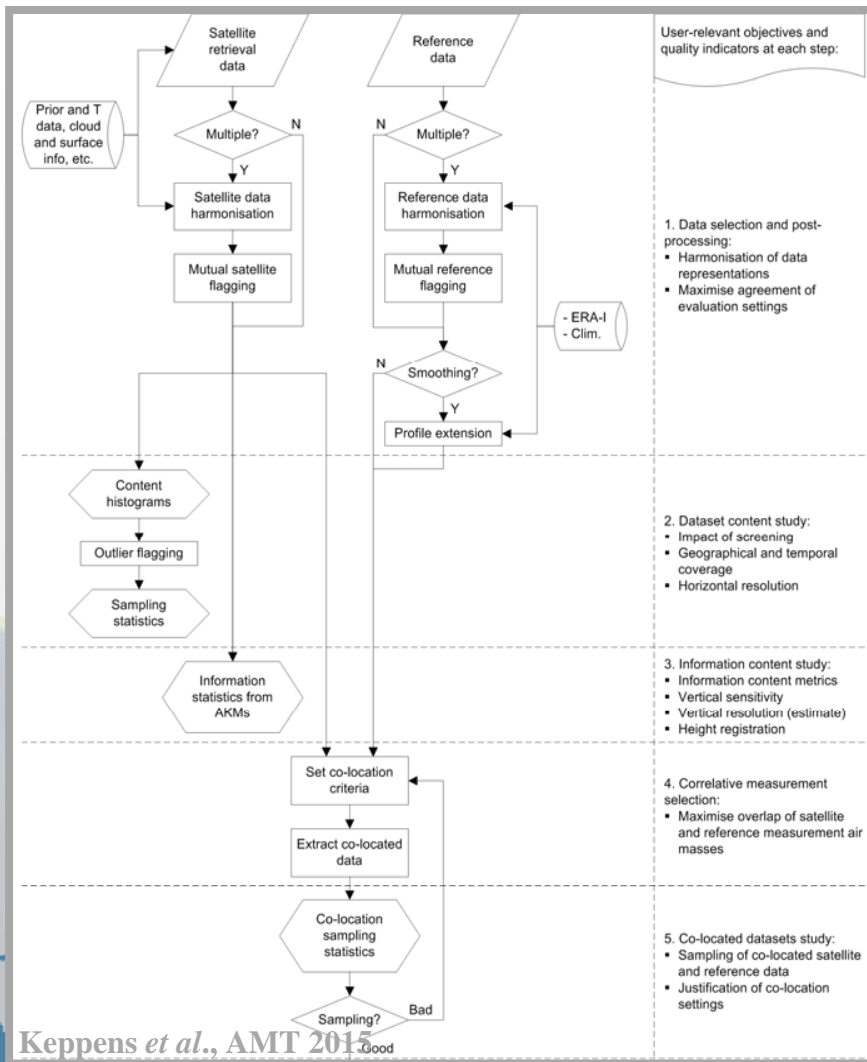
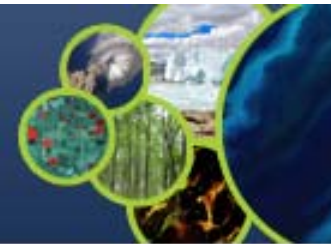


Discussed  
at ACC-10

AMTD  
paper  
accepted  
for  
publication  
in AMT  
last Friday

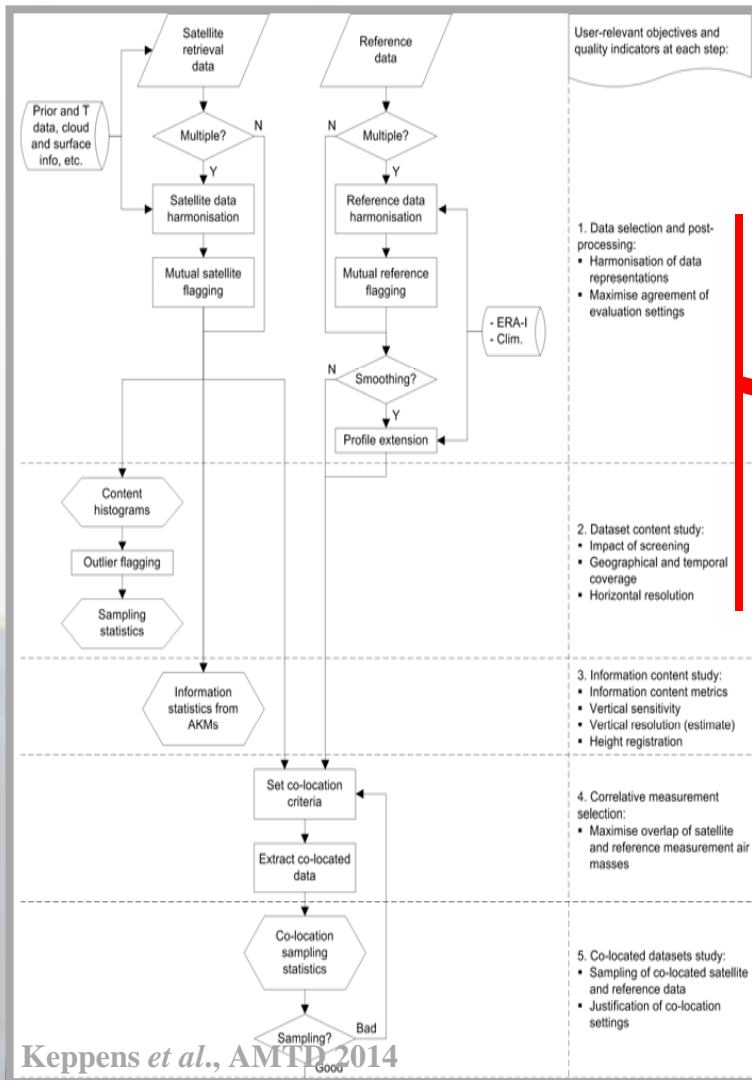
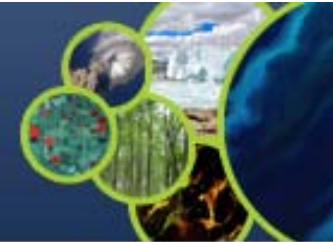
1. *Translation of user requirements into validation requirements*
2. Satellite data selection, filtering and post-processing
3. Data content study (DCS) of satellite dataset
4. Information content study (ICS) of satellite dataset
5. Selection and characterisation of correlative data
6. Identification and characterisation of co-located data pairs
7. Homogenization: Resampling, smoothing, and conversions of representation systems and units
8. Data comparisons: bias, spread, stability, dependences...
9. *Error budget of data comparisons => QA of ex-ante error bars*
10. Derivation of fit-for-purpose Quality Indicators
11. *QI based verification of compliance with user requirements*

# ESA CCI Ozone QA / Validation Process for Nadir Ozone Profile Retrievals



Keppens et al., AMT 2015

QA4CV type traceability chain of geophysical validation process

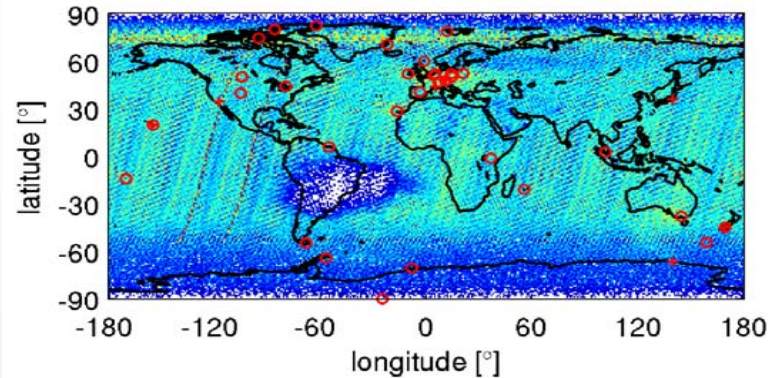


Keppens et al., AMTD 2014

## Post-processing, filtering...

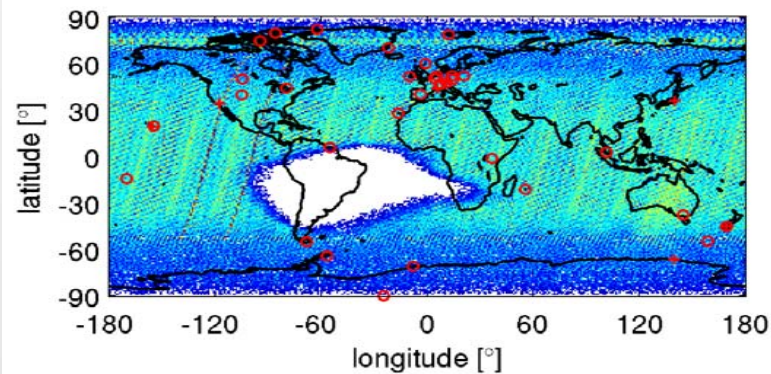
### Algorithm #1

OPERA v1.26 GC for GOME-2 2008



### Algorithm #2

RAL v2.1 GC for GOME-2 2008





# Information Content Studies

Analysis of vertical Averaging Kernels



## Information content

- Eigenvalues & eigenvectors of AKs
- (L)DFS
- Shannon IC, entropy
- Fisher IC / MQQ [Ceccherini et al., Opt. Exp., 2012]

## Vertical sensitivity

- Sum of row of AKs

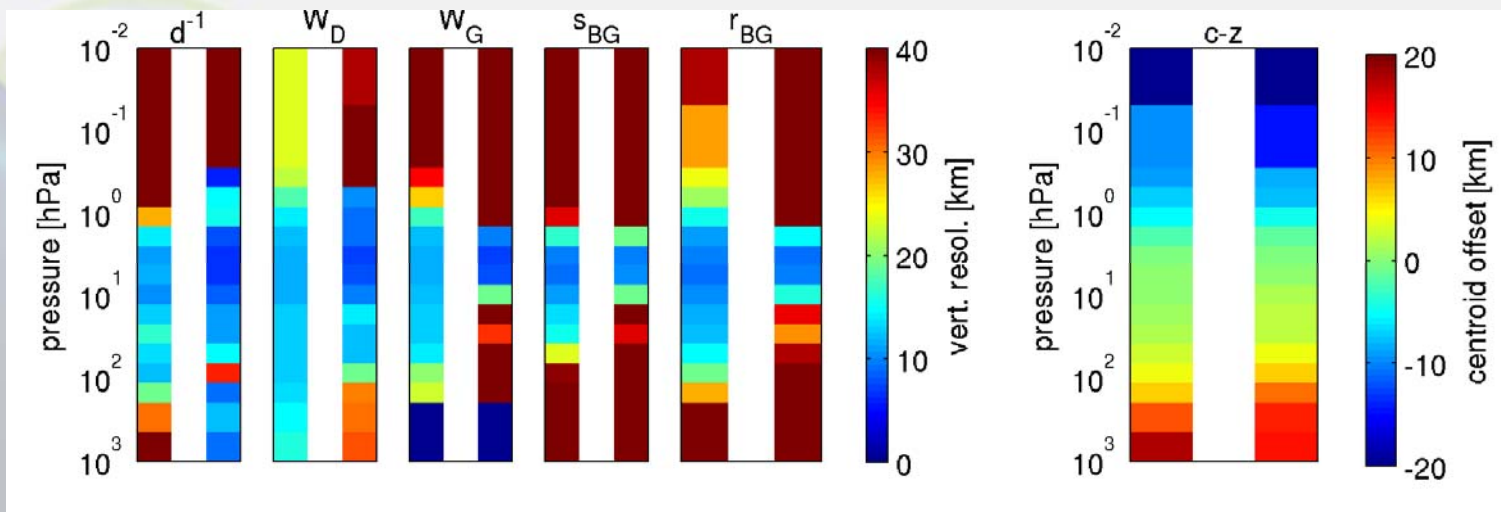
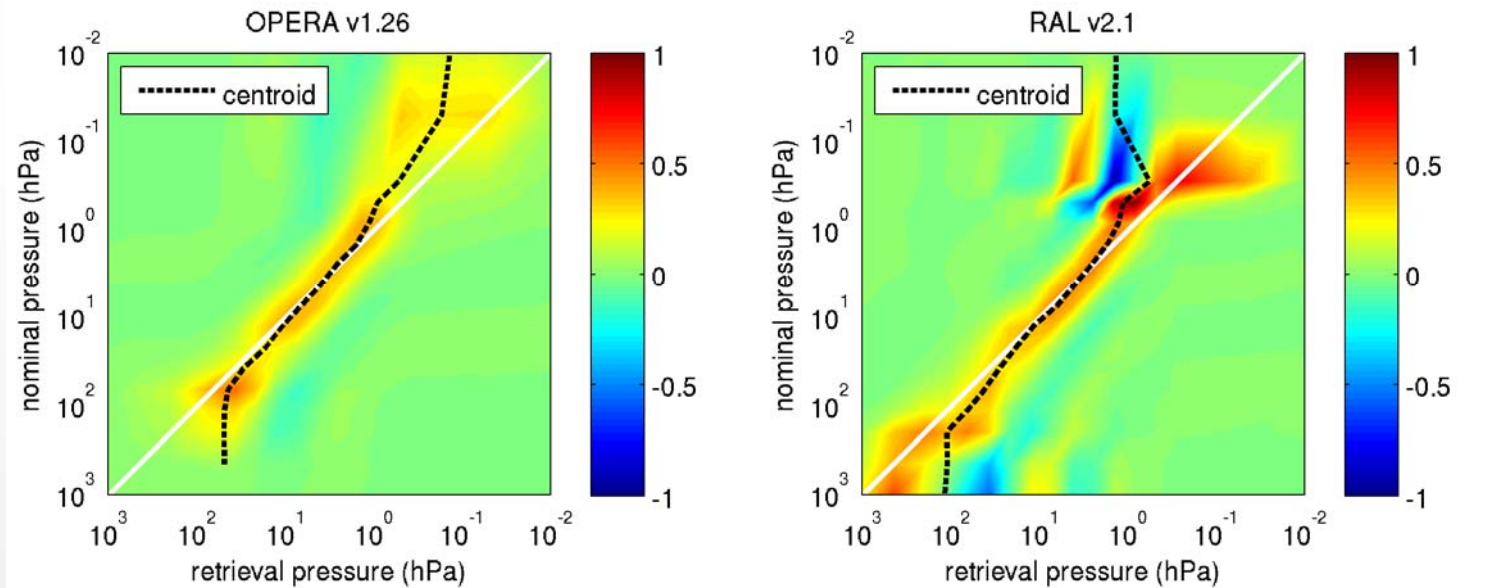
## Vertical resolution

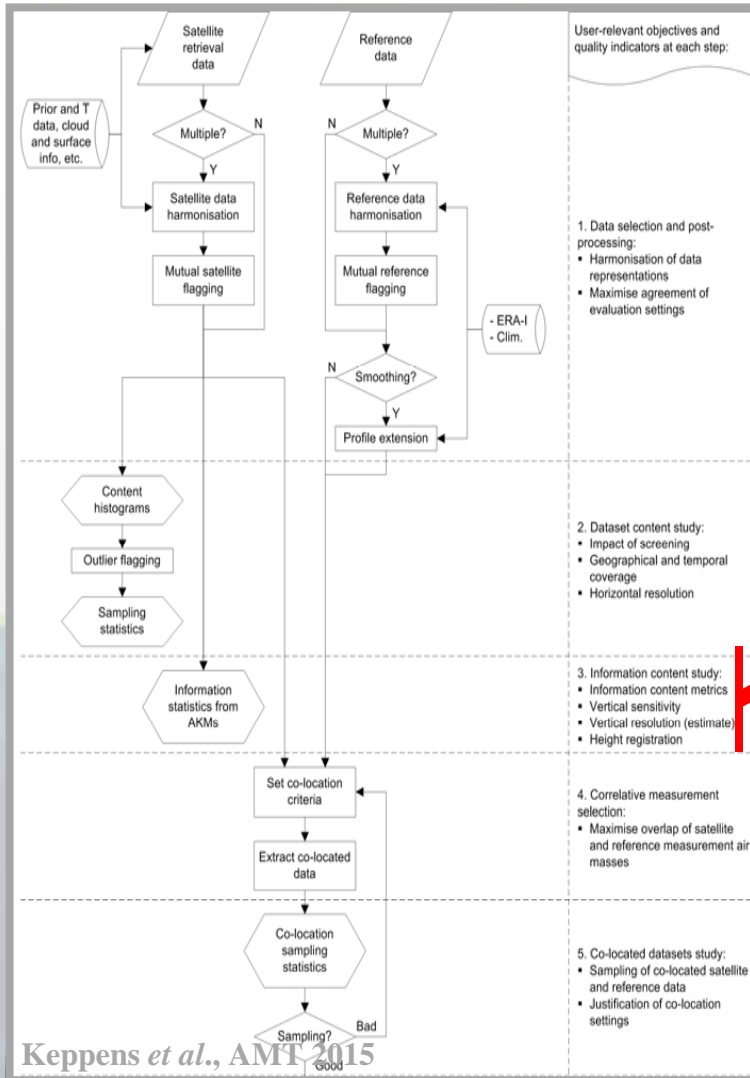
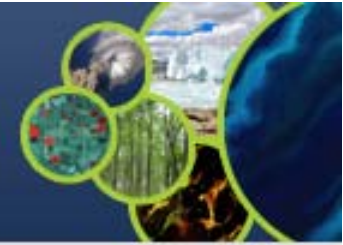
- Backus-Gilbert spread
- Other estimates

## Altitude registration

- Centroid





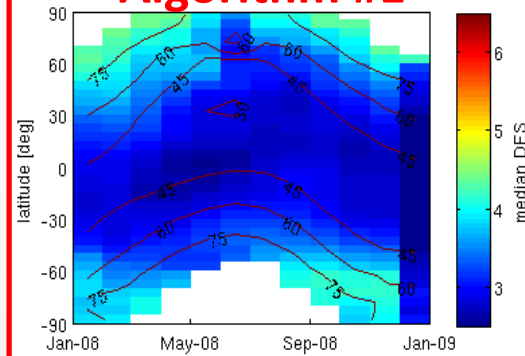


Keppens et al., AMT 2015

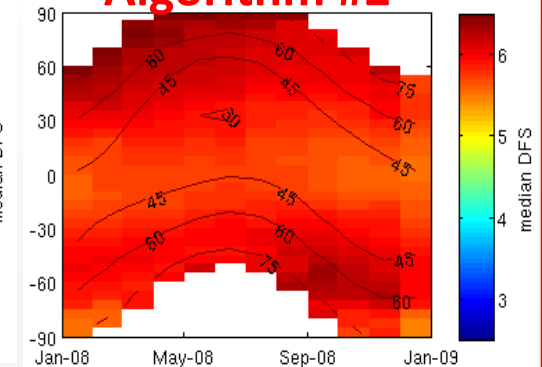
### Information content characterization

Pieces of independent information

**Algorithm #1**

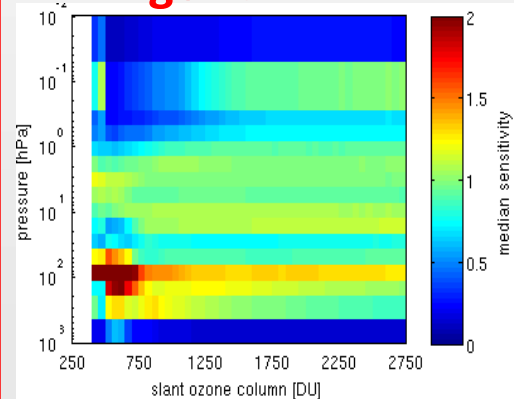


**Algorithm #2**

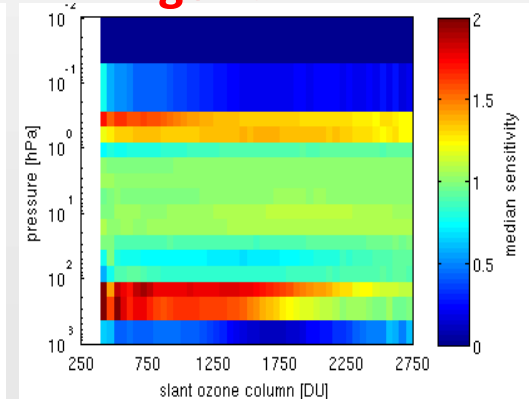


Dependence on ozone slant column

**Algorithm #1**

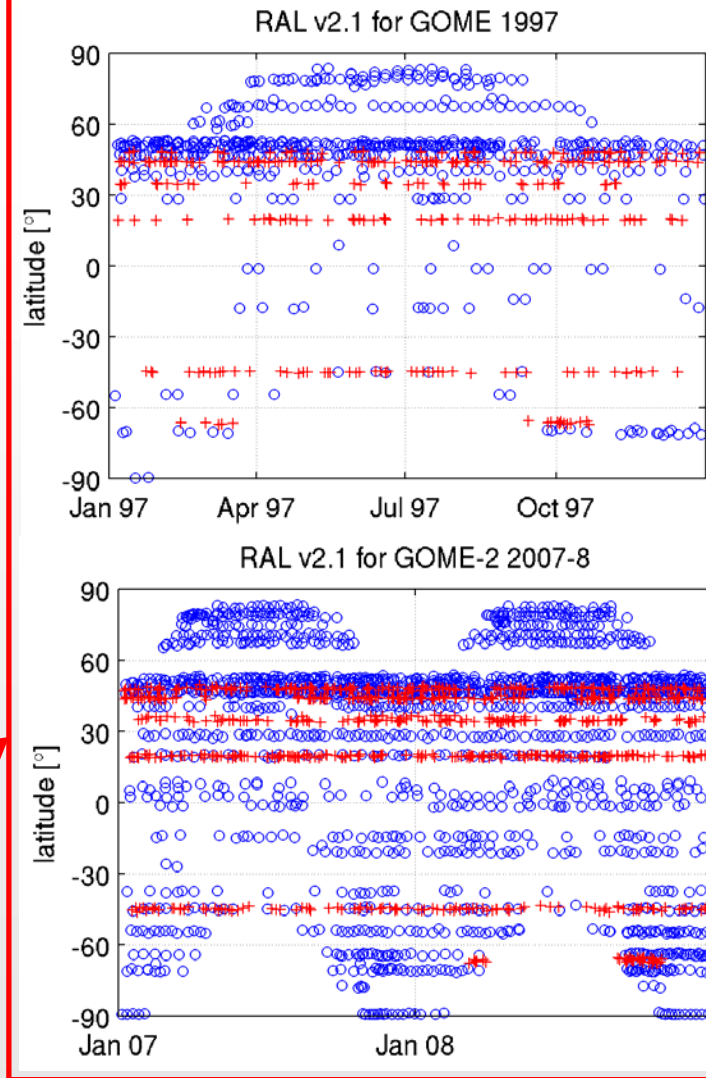
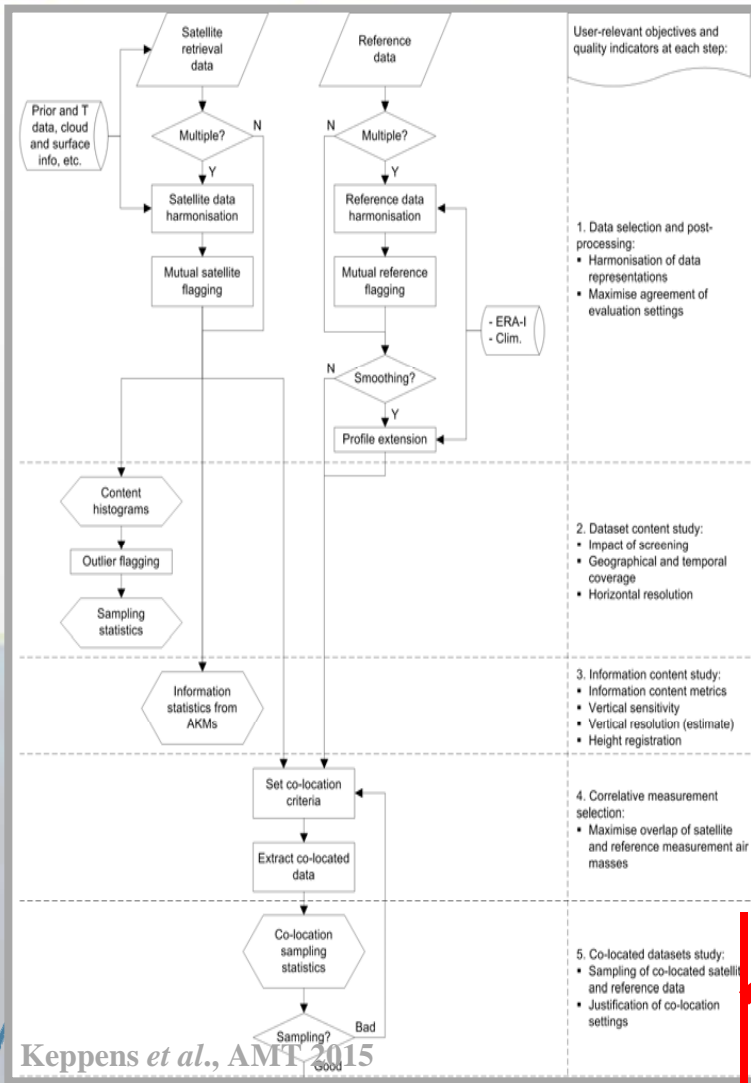


**Algorithm #2**



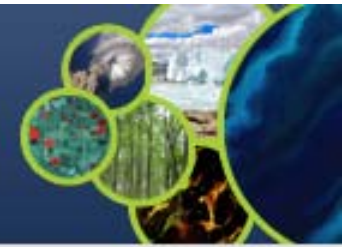
# Domain of application

## Co-location processing, analysis and documentation





# Resampling, smoothing, unit conversions.....

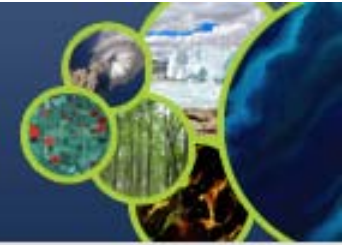


Profile:  $x' = M \times x$

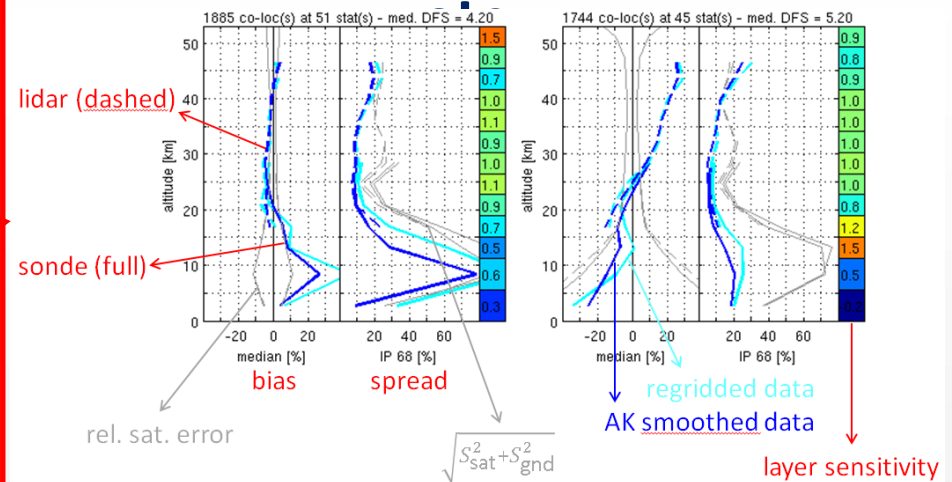
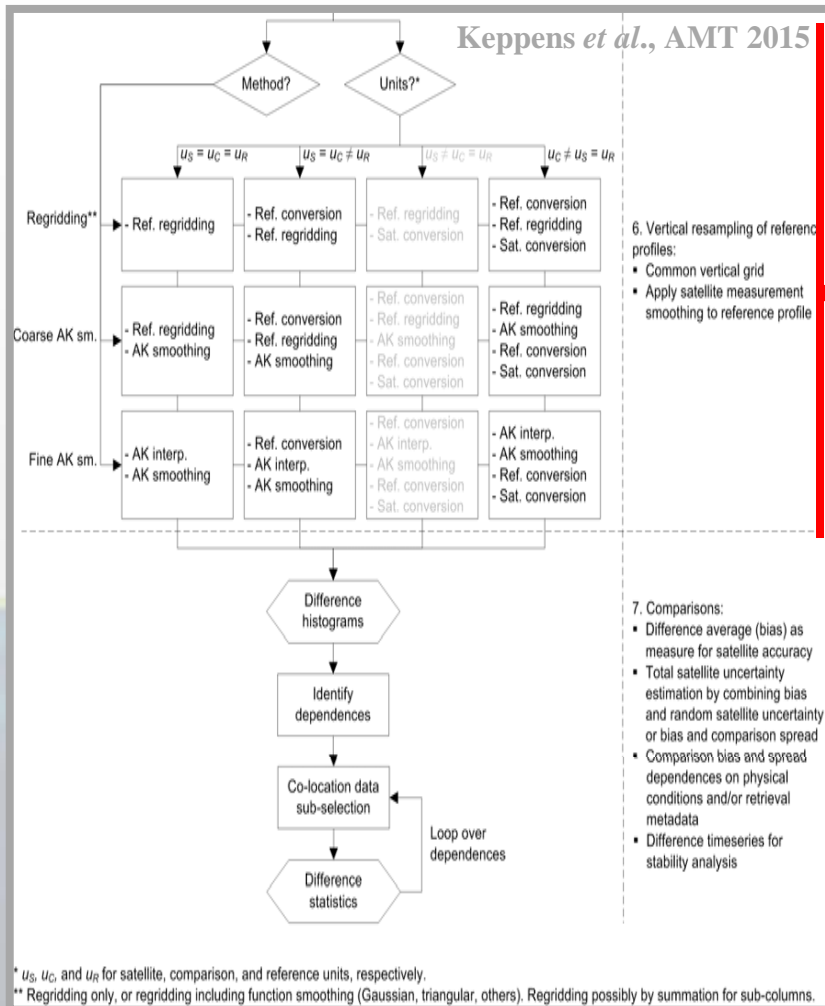
Covariance matrix:  $S' = M \times S \times M^T$

Several ways for averaging kernel matrix conversions...

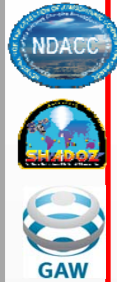
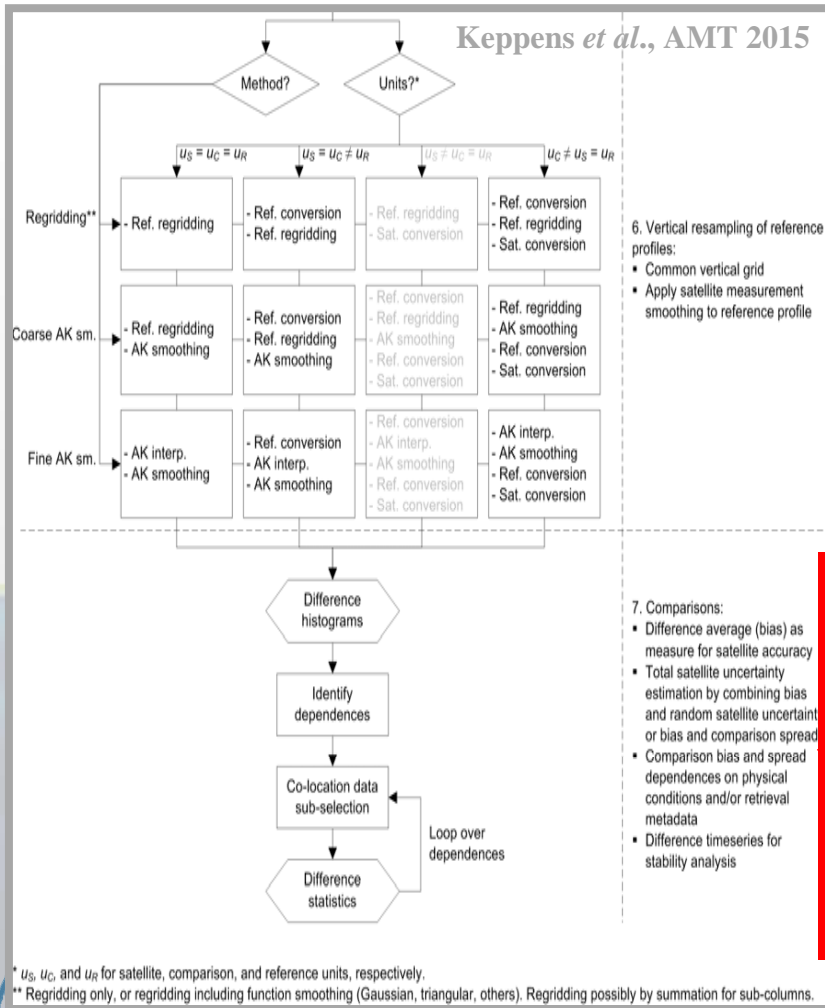
	Conversion from pressure and temperature profiles or vertical grid definitions	Conversion from available ozone profile vectors
VMR to ND Size: $N \times N$	$u \begin{pmatrix} T_1/p_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & T_N/p_N \end{pmatrix}$ (M1)	$\begin{pmatrix} x_1^{ND}/x_1^{VMR} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & x_N^{ND}/x_N^{VMR} \end{pmatrix}$ (M5)
ND to VMR Size: $N \times N$	$u \begin{pmatrix} p_1/T_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & p_N/T_N \end{pmatrix}$ (M2)	$\begin{pmatrix} x_1^{VMR}/x_1^{ND} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & x_N^{VMR}/x_N^{ND} \end{pmatrix}$ (M6)
VMR to PC Size: $L \times N$	$\frac{u}{2} \begin{pmatrix} \Delta p_1 & \Delta p_1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \Delta p_L & \Delta p_L \end{pmatrix}$ (M3)	$\begin{pmatrix} c_1 & c_1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & c_L & c_L \end{pmatrix}$ (M7) with $c_k = x_k^{PC} (x_i^{VMR} + x_{i+1}^{VMR})^{-1}$ for $k = i$
ND to PC Size: $L \times N$	$\frac{u}{2} \begin{pmatrix} \Delta z_1 & \Delta z_1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \Delta z_L & \Delta z_L \end{pmatrix}$ (M4)	$\begin{pmatrix} c_1 & c_1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & c_L & c_L \end{pmatrix}$ (M8) with $c_k = x_k^{PC} (x_i^{ND} + x_{i+1}^{ND})^{-1}$ for $k = i$



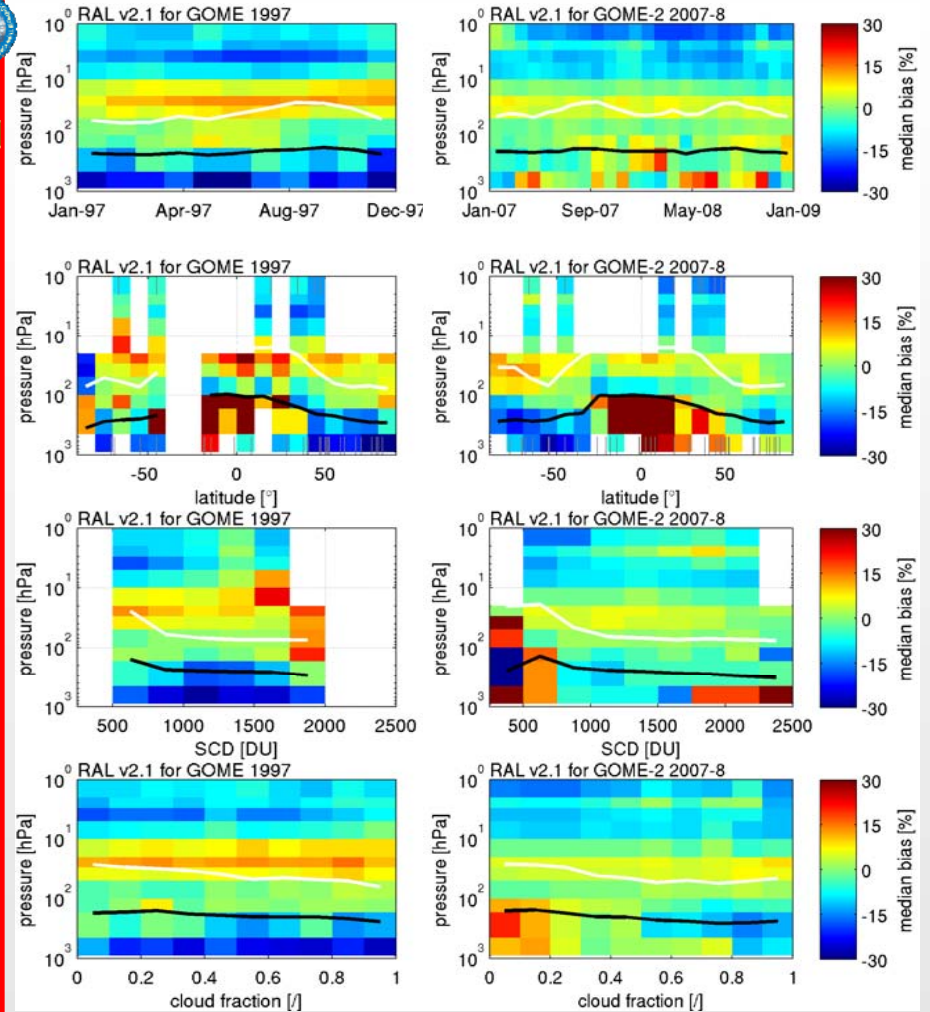
## Resampling, unit conversions



Different data manipulations and validation processes can provide different results, sometimes with complementary perspectives. It is often valuable (and more scientific) to apply and compare several methods rather than select only one !



## Data comparisons



# Validation reporting

## Compliance with user requirements



NADIR L2	Alt.	URD / PVP	GOME (1997)	GOME-2A (2007-2008)
Filtering			~ 3 %	~ 10 %
Geographical sampling			SAA and mid-Asia missing	SAA missing
DFS			5 to 5.5	5 to 6
Vertical resolution	TS	6 km to TS-col.	> 50 km	> 50 km
(resolving length estimate)	UT/LS	3 to 6 km	10 to 20 km	10 to 20 km
	MA	3 to 10 km	> 50 km	> 50 km
Height registration offset	TS		5 to 20 km (SZA dep.)	5 to 20 km (SZA dep.)
	UT/LS	/	negligible	negligible
	MA		-10 to -30 km	-10 to -30 km
Accuracy (bias)	TS		-10 to -30 % (-5 DU)	7 to 8 % (1 DU)
	UT/LS	/	-5 to 15 % (-2 to 5 DU)	1 to 4 % (1 DU)
	MA		-15 to 0 % (-3 to 0 DU)	-15 to 0 % (-3 to 0 DU)
Temporal dependence		/	Hardly any	Increased bias around and below TP for northern hemisphere winter
Meridian dependence	60-90		Negative bias around and below TP, small positive around ozone maximum	Negative bias around and below TP, positive around ozone maximum
	30-60	/	Negative bias below TP	Negative bias below TP
	0-30		Increased bias below TP	Increased bias below TP, related to bias for small SCD values
SCD dependence			Relation with meridian dependence less clear	Clearly related to meridian dependence
CF dependence			Slightly decreasing (more negative) bias with CF	Slightly decreasing (more negative) bias with CF
Comparison spread	TS		10 to 15 % (2 to 5 DU)	30 to 35 % (4 to 5 DU)
	UT/LS	/	5 % (3 DU)	5 % (3 DU)
	MA		5 to 10 % (0 to 3 DU)	5 to 10 % (0 to 3 DU)
Satellite random uncertainty	TS		10 to 40 %	10 to 30 %
	UT/LS	/	~5%	~5%
	MA		3 to 5 %	3 to 5 %
Total uncertainty	TS	10%	14 to 50 %	12 to 36 %
	UT/LS	8%	7 to 16 %	5 to 7 %
	MA	8%	3 to 18 %	3 to 18 %