Carbonyl Sulfide (OCS) Retrievals

Updated retrieval strategy to characterize Carbonyl Sulfide (OCS) homogeneously at sites at all latitudes using multiple FTIR within the IRWG. Based on recent work of Kremser et al., 2015; Lejeune et al., 2016; and Wang et al., 2016.

* **The primary goals are:**
	+ Characterize the tropospheric and stratospheric evolution of OCS using a priori and retrieval parameters as homogeneous as possible.
	+ Determine the the stratospheric OCS burden in the SPARC paper (Deshler et al.)
	+ Assemble a manuscript

This retrieval is based largely on Lejeune 2016. The primary difference is we have developed a zonal a priori and Sa based on global measurements from HIPPO and ACE which aids the strategy to be more latitude appropriate. This has been tested at a number of sites so far. Please submit data in standard IRWG HDF files.

* **Retrieval strategy for OCS**

See ftp://ftp.acom.ucar.edu/user/iortega/proj/ocs/ for files:

A priori profiles and Sa

 OCS\_HIPPO\_ACE.prfs

Sfit input files

 sb\_v8.ctl - shared

 sfit4\_v8.ctl – shared

 02026.691622-02058.728378\_hit12.hasc

 02026.691622-02058.728378\_hit12.hbin

references

Wang\_acp-16-2123-2016.pdf

Kremser\_et\_al-2015-Geophysical\_Research\_Letters.pdf

Lejeune\_JQSRT\_OCS\_2016.pdf

* 1. Micro-windows

Table 1 shows a summary of the recommended micro-windows used for the retrieval of OCS (Lejeune et al., 2016).

Table 1. Micro-windows recommended for the retrieval of OCS.

|  |  |  |
| --- | --- | --- |
| **Micro-windows [cm-1]** | **Column Gas** | **Profile Gas** |
| 2030.75 – 2031.06 (Optional) | CO2 | O3 |
| 2047.85 – 2048.24 |  | OCS, O3 |
| 2049.77 – 2050.18 | 16O12C18O | OCS, O3, CO |
| 2051.18 – 2051.46 | H216O | OCS, O3 |
| 2054.33 – 2054.67 | H218O, H216O | OCS, O3 |

* 1. Spectroscopy

Line parameters from HITRAN 2012. Others e.g. ATM16 and hot band lines (Lejeune 2016) were tested but found to have no significant improvement in fit, interference or retrieved column.

* 1. A priori and covariance information

A priori profiles and covariance zonal means have been created using airborne in-situ measurements during HIPPO (< 14km) and ACE-FTS (>14 km) measurements. The in-situ data set contains the results of analyses of discrete samples collected during all HIPPO Missions, 1 through 5 (Wofsy et al., 2012). The Missions took place from January of 2009 to September 2011. The stratospheric portion of OCS is obtained from ACE-FTS v3.5 between 2004-2103.

* Attached are the zonal data
* To account for the layer thickness and its influence please weight the Sa by (Sa/sqrt(thickness)) \*(Must do this)\*
* We used a Gaussian inter-correlation with a half-width length of 4 km for the off diagonal elements of the covariance matrix
	1. Uncertainties

Estimation of uncertainty in the retrieval of OCS is important and might be derived from OE in SFIT4 and/or PROFFIT. Below we have a short description of some errors we consider at MLO/Thule/Boulder.

For OCS we consider the line parameters, temperature profile, Solar Zenith

Angle (SZA), measurement noise, and instrumental line shape errors. Note that some type errors might be specific foe each site. A description for some errors is discussed below:

1. The systematic uncertainties in the line parameters are taken from the lower portion of the uncertainty range reported in HITRAN 2012. We use uncertainties for line intensity, air-broadened half width, and temperature dependence of the air-broadened half-width parameter. The uncertainty codes related to the peak absorption feature of the micro-windows shown in table 1 are the same: 2% for line intensity, 5% for air-broadened half width. The temperature dependence of the air-broadened half-width parameter is not reported but we assume 5%.

1. The error in the temperature profile might be different for each site. We quantify the error in the temperature profile by comparing radiosonde temperature profiles at or near each of our sites with the daily NCEP temperature profiles. The mean of the difference can be as the systematic component of the error, while the standard deviation of the difference can be viewed as the random component.
2. The error in the SZA is characterized by the pointing error of the instrument and the integration time. For our sites we have characterized the SZA error of 0.15 degrees and characterize this error as a random component.
	1. References

Kremser, S., N. B. Jones, M. Palm, B. Lejeune, Y. Wang, D. Smale, and N. M. Deutscher (2015), Positive trends in southern hemisphere carbonyl sulfide, Geophysical Research Letters, 42(21), 9473–9480, doi:10.1002/2015GL065879, 2015GL065879.

Lejeune, B., E. Mahieu, M. K. Vollmer, S. Reimann, P. F. Bernath, C. D. Boone, K. A. Walker, and C. Servais (2017), Optimized approach to retrieve information on atmo- spheric carbonyl sulfide (ocs) above the jungfraujoch station and change in its abundance since 1995, Journal of Quantitative Spectroscopy & Radiative Transfer, 186, 81 – 95, doi: http://dx.doi.org/10.1016/j.jqsrt.2016.06.001.

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Wofsy, S. C., B. C. Daube, R. Jimenez, E. Kort, J. V. Pittman, S. Park, R. Commane, B. Xiang, G. Santoni, D. Jacob, J. Fisher, C. Pickett-Heaps, H. Wang, K. Wecht, Q.-Q. Wang, B. B. Stephens, S. Shertz, A.S. Watt, P. Romashkin, T. Campos, J. Haggerty, W. A. Cooper, D. Rogers, S. Beaton, R. Hendershot, J. W. Elkins, D. W. Fahey, R. S. Gao, F. Moore, S. A. Montzka, J. P. Schwarz, A. E. Perring, D. Hurst, B. R. Miller, C. Sweeney, S. Oltmans, D. Nance, E. Hintsa, G. Dutton, L. A. Watts, J. R. Spackman, K. H. Rosenlof, E. A. Ray, B. Hall, M. A. Zondlo, M. Diao, R. Keeling, J. Bent, E. L. Atlas, R. Lueb, M. J. Mahoney. 2012. HIPPO Combined Discrete Flask and GC Sample GHG, Halo-, Hydrocarbon Data (R\_20121129). Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. <http://dx.doi.org/10.3334/CDIAC/hippo_012>