Froidevaux et al., GRL 33, L23812, doi:10.1029/2006GL027600, 2006

Auxiliary Material

Appendix A

Since MLS HCl is the primary focus of this work, we quantify here the sources of random and systematic errors that contribute to the uncertainty in retrieved abundances of MLS HCl. Supporting reference material not mentioned in the main paper is included.

The random error (precision) written in the MLS data files comes from a propagation of the MLS radiance (and a priori) errors through the MLS retrievals, described by Livesey et al. [2006]. This component should be the main contributor to uncertainties in temporal changes of HCl, such as the monthly-averaged near-global means shown in this work. The estimated single-profile precision for MLS HCl in the upper stratosphere agrees typically to within 20-40% with the standard deviation of HCl about its mean in a narrow latitude bin; for such analyses, we choose a (10 degree) tropical bin or a summer high latitude bin, in order to avoid regions of larger natural variability, such as high latitudes during winter or spring. The MLS upper stratospheric and lower mesospheric results shown in this paper apply to a vertical retrieval grid having 6 levels per decade change in pressure, or about 2.7 km spacing; however, the vertical resolution implied by the MLS averaging kernels is 5 to 6 km in this region, so adjacent retrieval levels will have a correlated response. This is caused partly by the MLS field of view (FOV), with half-power beamwidth of 1.5 km (for the 640 GHz MLS radiometer named R4, relevant to HCl), by line-of-sight ray trace smearing, and by smoothing applied in the vertical and horizontal direction during the 2-D along-track retrieval process. [Livesey et al., 2006]. We note that vertical smoothing should not lead to a smoothing of temporal variations, if such a variation (or decrease) occurs coherently on a vertical scale of about 5 km or more.

Table A.1 lists the sources of systematic error considered for the upper stratospheric and lower mesospheric HCl error budget, their magnitude, and the likely percent impact on retrieved HCl mixing ratios. A description of each systematic error source, following the tabulated list, is given below. Both pre-launch calibration assessments and post-launch analyses have contributed to these results. The total systematic uncertainty is taken as a combination (root sum of the squared contributions) of the individual error sources and is used in this paper as an error bar for the MLS monthly averages, since the purely random error is a negligible component of the error in such averages. Inasmuch as possible, we have attempted to use 2-sigma (or 95% confidence level) type errors; a 2 to 3-sigma type of error, or a maximum error, has been used in each of the components considered in Table A.1 The total combined error shown in Table A.1 amounts to 4.6%. We have chosen to use a slightly more conservative estimate of 5% as the MLS (systematic) error bar in the main paper. This can be applied as a total error for the monthly zonal means discussed in the paper (Figure 5), given the excellent precision (negligible random error) for such averages. However, temporal changes in HCl do not depend on the exact value of this systematic error estimate.

Antenna system transmission: Errors categorized in Table A.1 as antenna transmission come from imperfect knowledge of antenna transmission (or reflectivity), including ohmic losses as well as spillover and diffraction effects. The pre-launch calibration work described by Cofield and Stek [2006] details these sources of uncertainty and gives a radiometer-dependent radiance scaling uncertainty (3-sigma) of 0.38% for the relevant radiometer used to measure HCl. We use a more conservative (worst case) value of 0.8%, because post-launch calibration using moon scans and a moon thermal model do not preclude errors as much as 0.4% above the pre-launch values.

Radiometric calibration: MLS radiances are radiometrically calibrated every 24.7 s by views to cold space and an ambient calibration target, fast enough to accommodate drifts in raw signal counts. Radiometric calibration scaling error at the switching mirror is estimated to be 0.45% [Jarnot et al., 2006].

Sideband ratios: For each emission band region, knowledge of relative radiance contributions from the two frequency ranges providing signals to the MLS double-sideband system is needed. The uncertainty in this ratio is obtained from the peak-to-peak departures from a smooth fit to the measured sideband ratios as a function of channel. The band 13 (HCl) radiance error estimate of 0.25% in Table A.1 is based on the pre-launch analyses of Jarnot et al. [2006].

Channel filter shapes and position: The filter channel transmission properties have been characterized before launch, and the radiance uncertainty associated with a possible error in center position as well as filter shape is given as 0.3%, based on an upper limit from the work of Jarnot et al. [2006].

Standing waves: Post-launch scans of the moon with the MLS antenna have provided new information regarding spectral artifacts that appear in views through the limb port. These effects are believed to be caused by standing waves that can be generated by multiple reflections; such effects were noticed pre-launch [Jarnot et al., 2006], but are best characterized post-launch through the same optics as the atmospheric views. The moon scan data indicates that spectral artifacts exist at the 1% level (for radiances); such effects cannot be removed because they are sideband-dependent, but information in each sideband is combined by the EOS MLS double-sideband measurement system.

Gain compression: Another non-negligible source of error comes from gain compression in the amplifiers; modeling and laboratory analyses of this effect are continuing, with current estimates pointing to a spectral error of order +1% (the sign implies a small overestimate of HCl abundances).

FOV effects: The characterization of the three FOV error sources mentioned in Table A.1 comes from the pre-launch calibration results of Cofield and Stek [2006]. The first effect deals with the knowledge of the FOV direction (for MLS band 13 data), meaning knowledge of pointing relative to that obtained from tangent pressure and temperature retrievals using the 118 GHz radiometer (R1, measuring oxygen line emission). The uncertainty in the elevation difference between R1 and R4 views of the atmospheric tangent point is 0.004 degrees. This uncertainty corresponds to about 200 m at the tangent point, typically about 3000 km away from MLS. We translate this into a 0.7% percent error for HCl, based on typical HCl gradients in the upper stratosphere of no more than 0.1 ppbv/km and a typical HCl mixing ratio of 3 ppbv. The error in our knowledge of absolute pointing (and tangent pressure) derived from R1 is assessed primarily from possible uncertainties in the O2 spectral parameters, with linewidth being the main error source, as mentioned further down in Table A.1. The FOV shape effect comes from the 0.002 (or 0.2%) beam efficiency uncertainty and a 0.0015 degree uncertainty in the half-power beamwidth (HPBW) measurement [Cofield and Stek, 2006]; both of these effects should be small because the HPBW (for R4) is 1.5 km (smaller than the 2.7 km retrieval grid) and the beamwidth effect is largely normalized out in the radiance convolution. A 0.2% error in HCl is estimated for these effects. Finally, the FOV scan dependence was measured [Cofield and Stek, 2006] and a worst case (radiance) estimate (see Table A.1) of the impact of neglecting this effect is estimated by convolving this dependence with a radiance model for the MLS bands. The impact on HCl of neglecting this radiance effect in the forward model (as part of the MLS data processing) is estimated to be 0.6%, based on a typical 40 K HCl signal (and vertical gradient) for the upper stratosphere.

HCl spectroscopic parameters: Line positions and strengths are generally known very accurately at microwave frequencies, and each of these error sources is not expected to contribute more than 0.1% to the error budget; the line strength error comes from doubling the error in the dipole moment measurement [Kaiser, 1970], since line strength is proportional to dipole moment squared. Temperature errors can lead to retrieval errors through the line strength temperature dependence. We estimate the total impact of temperature inaccuracy further down in Table A.1; this includes effects from the radiative transfer source function and hydrostatic balance temperature dependences, as part of the forward model and the retrievals. The linewidth for HCl was measured pre-launch by Drouin [2004] with an estimated error of 3% for upper stratospheric temperatures; this agrees, within this error, with most previous laboratory data. The potential impact on HCl is estimated by analogy to the ozone results of Froidevaux et al. [1996].

Retrieved tangent pressure: For the tangent pressure retrieval accuracy, we use a 2% maximum error in the O2 linewidth (based on pre-launch laboratory data) as the main source of error. This translates to a 1% maximum error for upper stratospheric HCl, based on tests of the MLS HCl retrieval sensitivity to a change in O2 linewidth.

Retrieved temperature: The validation results shown in Froidevaux et al. [2006] indicate that the MLS temperature retrievals are within 1% (about 2.5K) of other measurements in the upper stratosphere and lower mesosphere. This should lead to errors in HCl of less than 2%.

Retrieval numerics and closure: Retrieval-induced biases have been estimated based on a pre-launch generation of simulated radiances and retrievals; we find that the HCl average error in terms of comparisons to the "true" (simulated) profiles, based on a full day simulation, is less than 1% in the upper stratosphere. Actual daily average radiance residuals for HCl are also typically of order 1% or less (see Read et al. [2006]). This does not mean that the HCl error cannot be larger than this, since the retrievals will tend to absorb (as HCl) error sources that produce a perturbation component correlated with the HCl spectrum. However, good radiance closure does help to build confidence in the overall retrieval process. Also, the work of Froidevaux et al. [2006] has shown that there is very good correlation in the spatial (latitudinal) gradients of MLS, HALOE and ACE (coincident) HCl measurements, despite the fact that the HALOE stratospheric values are systematically 10-15% lower than those from MLS and ACE.

Retrieval a priori influence: The influence of the a priori HCl field could lead to an error in retrieved HCl of 0.5% near 0.1 hPa, as the radiance signal-to-noise decreases. As for the UARS MLS retrievals, we have chosen large a priori errors (6 ppbv in the case of HCl) to reduce any biases from this effect. Error analyses, evaluating the measurement and a priori contributions using the retrieval and a priori uncertainty values, point to a small (< 0.5%) impact from the a priori; this has also been confirmed by the results of test retrievals that make use of a different a priori value.

Forward model approximations: The MLS forward model description is given in Read et al. [2006]. One estimate of potential errors in forward model approximations is obtained by comparing independent algorithms. Comparisons between the JPL and University of Edinburgh forward models for HCl yield radiance differences of less than 0.5 K, or 1.3% for HCl in the upper stratosphere.

We have considered other sources of error as well and mention these for completeness; they are not listed in Table A.1 because they are believed to have a negligible impact. For example, digitizer non-linearity effects on spectral calibration may contribute up to 0.02K or 0.05% error for HCl in the upper stratosphere. Also, power supply interactions can lead to spectral artifacts which could impact the radiances at the 0.05K level, or 0.1% for HCl, also negligible. The impact of vertical smoothing constraints for typical retrievals is also expected to be small, based on full day tests with and without smoothing, which indicate less than a 0.5% root mean square effect, and essentially zero effect for averaged results in the upper stratosphere and lower mesosphere; we would expect this kind of error to be negligible as a systematic effect for monthly averages. Finally, we can also neglect errors arising from contaminant species and continuum emission for HCl in the upper stratosphere, given the clean HCl spectrum at these heights and the good knowledge of ozone (the primary contaminant species for HCl), which is retrieved by MLS in various bands, with excellent (5 to 10%) comparison results versus several other validated data sets [Froidevaux et al., 2006].

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