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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Characteristics and error estimations of stratospheric ozone and ozone-related species over Poker Flat (65° N, 147° W), Alaska observed by a ground-based FTIR spectrometer from 2001 to 2003" *by* A. Kagawa et al.

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General Comments

This well-organized paper presents a detailed characterization and error analysis of first vertical profile and partial column retrievals performed on ground-based FTIR spectra recorded at the northern hemisphere mid-to-high latitude site of Poker Flat, Alaska. This work is complementary to recent literature on coarse vertical profiling of a

suite of trace gases from other FTIR sites of the NDSC/NDACC (e.g. Schneider et al., 2005, JQSRT; 2005, ACP; 2006, ACP, e.g. Barret at al., 2002, JGR; 2003, JGR; 2005, JQSRT, e.g. Wood et al. 2004, JGR, e.g. Rinsland et al., 2003, JGR). However, the authors omit many of these key references, which place their general work – and also their specific results – in a broader context.

Overall, this study reflects the trend of the ground-based FTIR community moving to well-characterized data products with detailed error budgets, which can be used in more rigorous comparisons with other observations, while taking into account different viewing geometries and sensitivities, etc. The authors present such a comparison (with sondes, TOMS, and HALOE data), and as such, their work is of interest to the wider ACP/D community. I recommend that it be published, provided that the concerns outlined below are addressed.

Specific Comments

Section 1:

Page 3, paragraph starting on line 3: A reference to Rinsland et al., 2003 (JGR) should be added and briefly mentioned as an example of a study of the stabilization of Cly using FTIR data from multiple NDSC/NDACC observation sites.

Page 3, paragraph starting on line 14: More recent references would be helpful in the introduction, both to the recent (optimal estimation-based) FTIR work mentioned in the General Comments above, and for the general atmospheric processes outlined for mid-latitudes.

Page 4, paragraph starting on line 7: In the beginning of the introduction, mid-latitude chemistry is alluded to, but later on in the intro (and summary) it is stated that Poker Flat is between mid-latitudes and the Arctic. Then, the following statement is made: "Because it is outside the polar vortex for most of the winter and spring, the gas phase and heterogeneous chemistry over Poker Flat is not affected by polar ozone loss, except

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for transport of diluted ozone from the polar vortex." This statement appears somewhat at odds with a recent paper by one of the co-authors (Kasai et al., 2005, Adv. Space Res.), where it is reported that "The winter to spring decrease of CO column over Alaska seems consistent with a strato-mesospheric vortex full of descending CO-rich air in winter and a CO-depleted air in spring when upward transport bring low CO from the mid-to-low stratosphere at high Northern latitudes." Thus, the stratospheric versus strato-mesospheric conditions over Poker Flat need to be addressed in more detail – if the authors have done back-trajectory or PV studies in the past, this work needs to be included or referenced. The location of Poker Flat in a mid/high latitude boundary region is precisely what is interesting, as the authors point out in the summary, but extra care is required in the interpretation of future results from this FTIR observation site, and this needs to be acknowledged.

Section 2:

P7, L13: It is not clear whether the ILS retrieved from the HBr cell measurement is only used as a diagnostic of instrument performance. Given that the authors use SFIT2 v.3.7, is it the “Simple phase error parameter” (IPHASE) that is being retrieved? Also, how often are HBr cell measurements made, and in what configuration (with the sun or a blackbody or globar source)? Details of instrument performance and stability (i.e. ILS monitoring) should be added to Section 2, while details of ILS retrievals (e.g. SFIT2 vs. LINEFIT), and how that information is used in trace gas retrievals (if at all) should be added to Section 3.

In other words, the authors need to describe the facilities and procedures that exist to measure the instrumental line shape of the FTS. How stable is the instrument over time? How exactly is this information included in or accounted for in the retrievals?

Section 3:

None.

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Section 4:

P8,L23: While the retrieval parameters and spectral fit microwindows may not be the same (or even very similar), it is nevertheless appropriate to also compare the O3, HCl and HF characterization results to those of Schneider et al. (2005, ACP). Furthermore, O3 results should also be compared with the detailed study presented in Schneider et al. (2005, JQSRT). HNO3 characterization results may additionally be compared to the more recent work of Wood et al. (2004, JGR).

Section 5:

Section 5.3: The error values reported in this study should be placed in the context of those reported by some of the investigators mentioned in the General comments, in addition to the work of Barret et al (2002, 2003, 2005), e.g. Schneider et al. (2005, JQSRT; 2005, ACP) for O3, HCl, and HF. The newer study of Wood et al. (2004, JGR) can also be used for HNO3. While it is not possible to simply compare the numbers (because every FTIR group makes some different assumptions in their retrievals, characterization and error analysis), including the numbers from other studies in Tables 4a-d (and perhaps highlighting the major differences in assumptions) would be helpful to the average reader. The discussion of the similarities/differences should be expanded.

Furthermore, the authors estimate ILS errors by varying the Effective Apodization Parameter (EAP), and therefore changing the modulation efficiency of the FTS. While this is a very good start, it is fair to point out that the current state-of-the-art in the NDSC/NDACC FTIR community is to estimate both modulation efficiency and phase errors of an FTS by using the LINEFIT algorithm of Hase et al. (1999, Appl. Opt.). Schneider et al. (2005, JQSRT; 2005, ACP) present a detailed analysis of the impact of modulation efficiency and phase errors on profile retrievals. In their 2005 ACP paper, phase error is the larger of the two, while both are still less than line intensity error (see Table 2). The authors should discuss the limitations of their approach, and any work

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already done to switch to higher SFIT2 versions, which allow one to use the modulation efficiency and phase error parameters produced by the LINEFIT algorithm from cell measurements.

Section 6:

P14,L10: It is difficult to judge the improvement after smoothing in the lower and middle stratosphere due to the large values below 10 km.

P14,L27: Schneider et al., 2005 (JQSRT) performs detailed FTS-O3-sonde comparisons, which account for the sonde errors. How does this work compare/differ? Please expand the discussion to include the relevant numbers from Barret et al. 2002/3 (Table 4 and/or Fig. 8) and from Schneider et al. (Fig. 15)

P15,L20: "HITRAN 2004 data are about 4% lower than the respective HITRAN 2000 lines." Something seems reversed in this paragraph... If the authors use HITRAN 2004 as default for the analysis in Fig. 5 (yes?), then switching to HITRAN 2000 would INCREASE the columns in Fig. 5 by about 4%, therefore widening the gap between FTS and TOMS. Please double-check the wording here.

Fig. 6: The slope and intercepts of Fig. 6 would give more quantitative information about the biases and differences in sensitivity between FTS and TOMS. Another thing to consider is that (at least for a mid-latitude site) 11% of the O3 total column is found below 10 km, where the sensitivity of the ground-based retrieval drops off quickly (Fig 2a). The retrieval information in this region is provided at least in half by the apriori (dofs = 0.5 between 0-12 km in Table 3a) and could be a source of non-negligible bias in the total column amounts if the a priori is incorrect by a large amount.

Section 6.3: Based on the discussion, it does not appear that the high-resolution HALOE data were smoothed by the FTIR partial column kernels before being compared. Given the non-ideal shape of the FTIR kernels for O3, HCl, and HF, this casts some doubt on the discussion of FTIR-HALOE biases, even though the a priori profiles

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of the g-b retrievals were HALOE-derived.

P17,L21: “Overall, the gb-FTS O3, HCl, and HF stratospheric columns are well correlated...” -> The R values of the scatter plots for HCl and HF are rather low ($R^2 = 0.29$ and $R^2 = 0.42$, respectively), therefore, I would agree that the qualitative features of the two datasets are similar (even though there appears to be a phase shift for HF); however, “well-correlated” seems too strong a statement. In addition to known HALOE biases (and possibly the authors not smoothing the HALOE profiles by the FTIR kernels), sampling differences will be responsible for a significant portion of the observed scatter. Plotting the ratio of HCl/HF may shed more light on the similarities and differences between FTS and HALOE.

Section 7:

Section 7.0: The authors indicated the use of monthly a priori (and monthly a priori covariances) (Section 3). This complicates the interpretation of the seasonal variations of the retrieved profiles shown in Figure 9. The change in the retrieved profiles should be compared to the change in the monthly apriori profiles used in the retrievals in order to account for this effect. If a single apriori profile was used, the seasonal cycles would be attenuated, but entirely attributable to changes in the real atmosphere.

Section 8:

“The retrieval errors were estimated in detail and used as the basis for discussion of seasonal and inter-annual variability in stratospheric ozone and ozone-related species.” -> The magnitude of seasonal variations in the partial columns (Section 7) was not compared to the error values (Section 5).

Finally, the wording of the other conclusions (TOMS, HALOE comparisons, etc.) may need to be revised, as per the detailed comments above.

Technical Corrections

Section 1:

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P3, L29 / P4,L1: What is the altitude of the Poker Flat site?

P4,L29: “For the purpose of (c), random and systematic errors of the retrieved species were calculated using formal error analysis procedures (Rodgers, 2000), and these species were compared with balloon-borne and satellite data.” -> Please re-word to clarify what is being done in this study (error budget, comparison with sondes and satellites) versus what is being done in other studies (comparison of results for other species with balloons and other satellites.)

Section 2:

P5, L14: “Two detectors, a mercury-cadmium-telluride (MCT) one and indium antimonide (InSb) one, were used for the spectral region.” -> “The instrument is equipped with Mercury Cadmium Telluride (MCT) and Indium Antimonide (InSb) detectors, which cover the ... and ... spectral regions, respectively.”

P5, L15: detecter -> detector

P5, L21: 3.051 cm^{-1} -> 3051 cm^{-1}

P5: Field-of-view information for each detector and/or filter would be a useful parameter to include for reference in Table 1.

P6, L21: forward models -> forward model’s

Section 3:

P7, L5: “measurement” -> “measurement noise” and remove the word “error” to be consistent with Rodgers’ terminology. Otherwise, “measurement ... error covariance matrix” refers to both S_ϵ here and S_M on P9.

P7,L6: (S_a and S_ϵ) -> (S_ϵ and S_a) so that the order matches the text.

P7, L8: Remove either the “and” or the “while”

P7, L11: “Diagonal elements of S_ϵ were taken to be covered 1-σ from the random noise

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of the observed spectra within the fitted spectral regions." -> "were taken from the 1-σ random noise in the measured spectra within the fitted spectral regions." –OR– is it that the noise is determined from the "typical 1-σ random noise of the spectral fits." ? Please clarify if this is the case. Also, how representative is, e.g. the value of SNR=200 for the entire ensemble of O3 spectra? In other words, is there much variation in the SNR of the recorded spectra?

General: Please explicitly state somewhere in Sect. 3, if not done already, that both S_a and S_ϵ are purely diagonal matrices.

P7, L18: "on ozone" -> "for ozone"

P7, L27: "The spectral absorption line shape also depends on temperature." -> The spectral absorption line shape depends primarily on pressure, while the line strength depends primarily on temperature.

Section 4:

P8,L10: Reword so that "calculated spectra are well-fitted to the observed spectra," and not the other way around.

Fig. 1: Can remove the four references to when the spectra were recorded from the caption, since this information appears in the figure. Should then add SZA information to the four figure panels. Reduce the number of significant digits in the %RMS value on the figures. Discuss in the manuscript how a threshold value of, e.g. 1.5% is arrived at for the rejection of spectra from the analysis of seasonal cycles.

Section 5:

P9,L10: Rodgers (2000) reserves the term "retrieval error" to mean the sum of "forward model error," "model parameter error," and "retrieval noise." Consider revising "total retrieval error" to, e.g. "total error."

P9,L20: Briefly mention the limitations of using S_a in Equation 6.

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P10,L26: “ray-tracing algorithm” -> “ray-tracing algorithm, which computes airmasses, as well as density-weighted temperature and pressure profiles. This means...”

P11,L18: Was the EAP a constant function of the optical path difference, or did it, e.g. decrease linearly from 1 at zero path difference to 0.9 at maximum path difference in the FTS?

Section 6:

Figure 3: Middle panels of a,b,c,d: pink and red are not easy to distinguish; furthermore, the plots spill onto the right panels with the averaging kernels, and the x-axis labels overlap. Using solid vs. dashed lines of one colour would improve things.

Figure 4: The x-axis range may be changed to display the peak differences below 10 km too.

P15,L14: “blue symbol” -> “blue symbols”

P15,L28: please clarify if all spectroscopic parameters were changed by 5%, not just the line strength, and in which direction for the air broadening and the temperature dependence of the half width (for those unfamiliar with details of differences between HITRAN 2000 and 2004).

P16,L6: “HALOE derived” -> HALOE-derived

Section 7:

None.

Section 8:

P19,L24: “averaging kernels functions” -> averaging kernel functions

P21,L3: “while” -> and

P21,L3: “the all” -> all

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