Importance of FOV Integration for ACE

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Background
While studying HDO/H$_2$O fractionation in tropical ACE spectra, using the JPL GFIT algorithm, we encountered two problems:
1. The retrieved H$_2$O & HDO profiles were dryer than expected in the tropical troposphere (a factor 2 at 10 km, worse lower), a problem also reported by Wayne Evans at last ACE meeting
2. Spectral fits to H$_2$O and HDO lines exhibited abnormal systematic residuals

Could these two problems have a common origin?
Example of abnormal spectral residual: strong $\text{H}_2\text{O}$ line at 18 km altitude

Positive residual where $T \sim 5-10\%$

Compensatory negative residual

Compared to:

Compensatory negative residual
Example of abnormal spectral residual: weak HDO line at 8.5 km altitude
Why is FOV Integration necessary?

Due to the 1.25 mrad diameter of the ACE external field of view (FOV), the radiation entering the instrument from the upper and lower parts of the FOV has traversed the atmosphere at different altitudes and has different radiance spectra.
Comparison of external FOV’s for solar occultation FTS

<table>
<thead>
<tr>
<th></th>
<th>FOV (mrad)</th>
<th>Altitude (km)</th>
<th>Distance to TP (km)</th>
<th>$Z_{FOV}$ (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATMOS</td>
<td>1.0 1.4 2.0</td>
<td>300</td>
<td>2000</td>
<td>2.0 2.8 4.0</td>
</tr>
<tr>
<td>MkIV</td>
<td>3.6</td>
<td>36</td>
<td>450</td>
<td>1.62</td>
</tr>
<tr>
<td>ACE</td>
<td>1.25</td>
<td>650</td>
<td>3000</td>
<td>3.75</td>
</tr>
</tbody>
</table>

Due to its higher altitude orbit, the ACE field of view subtends a larger range of altitudes ($Z_{FOV}$) at the limb than ATMOS or MkIV.

So although ATMOS and MkIV may neglect the FOV integration, ACE may not.
FOV Center Approximation

Many remote sensing retrieval algorithms have forward models that implicitly assume a linear variation of incident radiance with zenith angle, so that the FOV-center radiance provides a good approximation to the average FOV-integrated radiance.

Under this assumption, only the FOV-center ray need be considered, avoiding the computational cost/complexity of a proper integration of the incident radiance over the FOV.

This FOV-center approximation is usually very good, except for:
• saturated absorption lines
• cases where the vertical extent of the FOV at the tangent point exceeds the scale height of the predominant absorbing gases
Consider a single frequency: \( k_\nu = 0.3 \times 10^{-23} \text{ cm}^{-1}/(\text{molec.cm}^{-2}) \)
How the FOV integration smoothes the limb transmittance

- FOV-Center Transmittance (green line)
- FOV-Integrated mean transmittance (orange dotted line)

- Large dry-bias
- Small (<5%) wet-bias

Tangent altitude (km)

Limb Transmittance
Worst-Case Scenario – Tropical H$_2$O

H$_2$O vmr = 2% near the surface; 3 ppm at 16 km (tropopause) Additionally, pressure falls by an order of magnitude, [H$_2$O] decreases by 5 orders-of-magnitude (H$_{H_2O}$=1.25 km)

At tangent altitudes below 15 km, the H$_2$O limb opacity will change by a factor $e^{-(3.75/1.25)}=20$ across the ACE FOV.

Limb transmittance will change even more due to Beer’s Law: A spectral frequency that has a 65% transmittance at the top of the FOV will have a transmittance of 11% in the center of the FOV and 2% at the bottom -- a factor 30 change in radiance.

Thus the FOV-averaged transmittance (~18%) exceeds the FOV-center transmittance by a factor ~1.5. Neglect of the finite FOV should cause a factor ~1.5 under-estimate in H$_2$O.
Considering Multiple Frequencies
Examples of spectral residual resulting from neglect of FOV integration

In the following slides, the left-hand panels show spectral fits that result when the FOV integration is neglected.

The right-hand panels show the improvement resulting from a numerical FOV integration.
Ratio: 1-ray / 5-ray = 1.015

Ratio: 1-ray / 5-ray = 1.004
Ratio: 1-ray / 5-ray = 0.993

Ratio: 1-ray / 5-ray = 0.994
Ratio: 1-ray / 5-ray = 0.972

Ratio: 1-ray / 5-ray = 0.990
Ratio: 1-ray / 5-ray = 0.904

16.8 km altitude

15.5 km altitude

Ratio: 1-ray / 5-ray = 0.735
Retrieved $\text{H}_2\text{O}$ profiles with (red) and without (blue) FOV integration

**Upper Panel:**
5-ray FOV integration produces slightly drier $\text{H}_2\text{O}$ profiles above 20 km but much wetter below

**Lower Panel:**
Retrieval error (from rms spectral fits) is better at all altitudes with the 5-ray FOV integration
Ratio: 1-ray / 5-ray vmr profiles

Neglecting FOV integration causes:
- Small overestimate of H₂O in stratosphere
- Large under-estimate of H₂O in the troposphere
- Worse retrieval uncertainties at all altitudes
Important Clarification

I’m not saying that the archived ACE H$_2$O profiles are wrong by a factor 2 in the tropopause.

The magnitude of the tropospheric dry bias depends on the degree of saturation of the selected H$_2$O lines.

The ensemble of H$_2$O lines that I used, produced a factor 2 error due to neglecting the FOV integration.

The ACE H$_2$O lines are weaker than the ones that I chose, in which case the tropospheric dry bias will be smaller.

But, the best (i.e., T-insensitive, parent isotopolog) H$_2$O lines do become highly saturated in the troposphere.
Impact of FOV integration (or neglect thereof) on CO$_2$ is much less than on H$_2$O, especially in the troposphere.

Skews retrieved CO$_2$ profiles, relative to single-ray approach, but improves uncertainties.

Like H$_2$O, magnitude of impact likely depends on how strong are the selected CO$_2$ lines.
FOV integration is necessary whenever there is a non-linear variation of radiance vertically across the FOV such that the spectrum at the center of the FOV is not a good representation of the FOV-averaged spectrum. This can be caused by:

• Weak absorbers whose vmr varies exponentially with altitude
• Strong, uniformly-mixed absorbers (due to Beer’s law $e^{-k.x}$)

This effect is quadratic in the width of the FOV, so the impact on ACE data will be $(3.75/1.62)^2 = 5x$ worse than on MkIV
Conclusions (2)

The finite FOV width causes also distortion of the spectral line shapes because:
- At frequencies where the limb path is nearly opaque, photons come exclusively from the upper part of the FOV.
- At frequencies where the limb path is fairly transparent, photons come more equally from the all parts of the FOV.

Thus, in the vicinity of a strong line, the effective tangent altitude will be higher in the line center than in the line wings. For H$_2$O, with a tropospheric scale height of only 1¼ km, this altitude ambiguity can cause a large retrieval error.

Although strong H$_2$O lines can be ignored for the purposes of doing H$_2$O retrievals, their large residuals nevertheless upset retrievals of other gases whose absorption lines in the vicinity...
Side-Effect: Neglecting FOV integration smooths the retrieved vmr profiles

Difference Jacobian has zero area (hence no bias in retrieved vmr) and strong anti-correlation between tangent level and adjacent levels.

Difference Jacobian resembles (2’nd difference) smoothing constraint. Hence, use of single-ray Jacobians smoothes the retrieved vmr profile.

When Chris Boone switched from single-ray to 11-ray forward model, this implicit smoothing constraint disappeared, resulting in increased noise sensitivity when retrieval grid \( \Delta z = \) tangent altitude \( \Delta z < 3.75 \) km.
Summary – Impact of neglecting FOV Integration

Under-estimates tropospheric H$_2$O, esp. for saturated lines
- Avoiding saturated lines minimizes impact, but this is difficult
  (e.g. within ACE bandpass, lower tropospheric H$_2$O lines are either saturated, isotopologs, or T-sensitive)

Over-estimates unsaturated lines (e.g. stratospheric H$_2$O)

Systematically distorts spectral line shapes (and hence residuals) for strong lines.

These systematic residuals indirectly affect other species whose absorption lines are blended with strong H$_2$O lines.

Small effect on uniformly mixed gases, e.g. CO$_2$

Provides implicit smoothing constraint
Additional Material

Spectral fits to the HDO line used in figure 3 of Boone et al. [2007], with and without the FOV integration.

8.5 km tangent altitude spectrum from sr10909

1-ray, i.e. no FOV integration

5-ray FOV integration

11% HDO increase using 5-ray FOV