4. Retrieval – Principle and Method

4.1 SMILES observation species
4.2 Forward model development
4.3 Retrieval algorithm
4.4 Error analysis
4.5 SMILES observation capability
**SMILES observations**

**Standard Products**
- O$_3$, HCl, ClO
- HO$_2$, HOCl
- O$_3$ isotopes, BrO
- HNO$_3$, CH$_3$CN

**Research Products**
- UT/LS region (O$_3$, HCl, CH$_3$CN)
- Upper stratosphere and lower mesosphere (O$_3$, HCl, HO$_2$)
- UTH, Cirrus Cloud
- H$_2$O$_2$
- Isotope species of HCl, and CH$_3$CN
- Mass–Independent Fractionation of Ozone isotopes
**SMILES observation altitude range**

<table>
<thead>
<tr>
<th>Observation Altitude Range</th>
<th>Species</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mesosphere</strong> (medium/low SNR)</td>
<td>( \text{O}_3, \text{H}^{37}\text{Cl}, \text{H}^{35}\text{Cl}, \text{wind,} \text{OOO}^{18} \text{HO}_2, \text{OOO}^{17}, \text{ClO} ) ( \text{H}_2\text{O}_2 )</td>
</tr>
<tr>
<td><strong>Stratosphere</strong> (high SNR)</td>
<td>( \text{O}_3, \text{H}^{37}\text{Cl}, \text{H}^{35}\text{Cl}, \text{H}_2\text{O}, \text{ClO} ) ( \text{Temp, Pointing offset} )</td>
</tr>
<tr>
<td><strong>Stratosphere</strong> (medium/low SNR)</td>
<td>( \text{wind, HOCl, N}_2\text{O, CH}_3\text{CN, OOO}^{18}, \text{OOO}^{17} \text{HNO}_3, \text{HO}_2, \text{BrO, H}_2\text{O}_2, \text{SO}_2 )</td>
</tr>
<tr>
<td><strong>UT/LS</strong></td>
<td>( \text{H}_2\text{O, Ice water content, O}_3 )</td>
</tr>
</tbody>
</table>
SMILES has 3 observation frequency bands. Simulated Observation Spectrum are shown with each molecule and at each tangent height.

- 2 spectrometers of 1200 MHz bandwidth
- 1.8 MHz resolution
### Products by JEM/SMILES experiment

<table>
<thead>
<tr>
<th>Processing modes</th>
<th>Band A</th>
<th>Band B</th>
<th>Band C</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stratospheric</strong>&lt;br&gt;high SNR&lt;br&gt;10-60 km</td>
<td>O$_3$, H$^{37}$Cl, H$_2$O, Temp, Pointing offset</td>
<td>O$_3$, H$^{35}$Cl, H$_2$O, Temp, Pointing offset</td>
<td>H$_2$O, ClO</td>
</tr>
<tr>
<td><strong>Stratospheric</strong>&lt;br&gt;medium/low SNR&lt;br&gt;10-60 km</td>
<td>wind, HOCl, CH$_3$CN, OOO$^{18}$, HNO$_3$, BrO, H$_2$O$_2$, SO$_2$</td>
<td>wind, N$_2$O, OOO$^{18}$, HO$_2$, HNO$_3$, SO$_2$</td>
<td>O$_3$, OOO$^{18}$, OOO$^{17}$, HO$_2$, HNO$_3$, BrO</td>
</tr>
<tr>
<td><strong>Mesospheric</strong>&lt;br&gt;medium/low SNR&lt;br&gt;50-90 km</td>
<td>O$_3$, H$^{37}$Cl, wind, OOO$^{18}$, H$_2$O$_2$</td>
<td>O$_3$, H$^{37}$Cl, wind, OOO$^{18}$, HO$_2$, SO$_2$</td>
<td>HO$_2$, OOO$^{18}$, OOO$^{17}$, ClO</td>
</tr>
<tr>
<td><strong>UT/LS</strong></td>
<td>H$_2$O, Ice water content, O$_3$</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Extremely Low SNR</strong></td>
<td>H$_2$CO, HOBr, ClONO$_2$, OCIO, ClOOCI, H$_2$SO$_4$</td>
<td>CH$_3$Cl, H$_2$CO, HOBr, ClONO$_2$, OCIO, ClOOCI</td>
<td>COF$_2$, ClONO$_2$, NO$_2$, OCIO, ClOOCI</td>
</tr>
</tbody>
</table>

blue: single scan, red: daily average, green: monthly average, black: very challenging
System model

Forward model development

1) radiative transfer model
2) Sensor model

$L1 \text{ Data} = S + B_{\text{mole}} + T_{\text{sys}}$

- $S$: Signal from purpose molecule in the atmosphere
- $B_{\text{mole}}$: Background Base line from molecules (O3, H2O, N2, O2, etc.)
- $T_{\text{sys}}$: System noise ($T_{\text{ant}}$, $T_{\text{opt}}$, $T_{\text{rx}}$) + Side lobe

L1 data

Temperature calibration

Hot load: emission from side lobe
Cold load: emission from side lobe

Signal of limb observation

$T_{\text{b}}^*$

$T_{\text{sys}}$ ($T_{\text{ant}}$, $T_{\text{opt}}$, $T_{\text{rx}}$)
$T_{\text{ant}}$: antenna noise temperature
$T_{\text{opt}}$: optics noise temperature
$T_{\text{rx}}$: receiver noise temperature
Radiative transfer process in the atmosphere

Items included

- Atmospheric Refraction is included
- Line shape function is used: the Voight functions for each pressure.
- Continuum Liebe MPM89 for operational code, SMILES continuum for research code
- 2 dimension integrals are possible for the atmospheric models in research code
- Scattering calculation included in research code
Radiative transfer calculation including cloud cases for research products
An example: Ice cloud effects in the UT/LS

Example: Effects of cirrus in different ice water path on SMILES spectra

(SetUp: tropical standard atmosphere, cirrus 12–13km, effective size 12mm, 4km tangent altitude)
Radiative transfer calculation in the atmosphere

Atmospheric Continuum in SMM region

Difference of absorption of the several models are more than 50%
Laboratory Experiment of water vapor
TDS spectrometer + SMILES SIS spectroscopy

Continuum model applicable to SMILES
Continuum model applicable to SMILES

Laboratory Experiment of water vapor
TDS spectrometer + SMILES SIS spectroscopy
## Summary of SMILES molecular spectroscopic data

<table>
<thead>
<tr>
<th></th>
<th>Freq. (GHz)</th>
<th>γ</th>
<th>n</th>
<th>Current Accuracy</th>
<th>Required Accuracy by the error analysis</th>
<th>Priority</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>O₃</strong></td>
<td>625.372</td>
<td>2.99</td>
<td>0.75</td>
<td>4%</td>
<td>1%</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>650.732</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>1%</td>
<td>1</td>
</tr>
<tr>
<td><strong>H³⁵Cl</strong></td>
<td>625.919</td>
<td>3.41</td>
<td>0.73</td>
<td>4%</td>
<td>1%</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Pressure Shift $\delta_0$(MHz/Torr)=0.146, s=0.4047, $\chi$=0.3763) 17.8%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>H³⁷Cl</strong></td>
<td>624.978</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>1%</td>
<td>2</td>
</tr>
<tr>
<td><strong>ClO</strong></td>
<td>649.451</td>
<td>2.782</td>
<td>0.86</td>
<td>3%</td>
<td>1%</td>
<td>2</td>
</tr>
<tr>
<td><strong>HO₂</strong></td>
<td>625.660</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>649.702</td>
<td>3.51</td>
<td>0.63</td>
<td>4%</td>
<td>3%</td>
<td></td>
</tr>
<tr>
<td><strong>H₂O₂</strong></td>
<td>625.04</td>
<td>3.78</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>3</td>
</tr>
<tr>
<td><strong>HOCl</strong></td>
<td>625.076</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>1</td>
</tr>
<tr>
<td><strong>O₃ isotopes</strong></td>
<td>Many</td>
<td>---</td>
<td>---</td>
<td>0.5%</td>
<td>1%</td>
<td>1</td>
</tr>
<tr>
<td><strong>BrO</strong></td>
<td>624.768</td>
<td>3.05</td>
<td>0.80</td>
<td>3%</td>
<td>5%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>650.179</td>
<td>3.03</td>
<td>0.80</td>
<td>3%</td>
<td>5%</td>
<td></td>
</tr>
<tr>
<td><strong>HNO₃</strong></td>
<td>624.484</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>1%</td>
<td></td>
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<tr>
<td></td>
<td>624.776</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td></td>
<td>625.345</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td></td>
<td>650.288</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td><strong>CH₃CN</strong></td>
<td>624.819</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>624.926</td>
<td>---</td>
<td>---</td>
<td>3%</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

*Summary Note:* The table above lists various molecules along with their respective frequencies (Freq.), γ values, and accuracy levels among others. This data is crucial for forward model development as it provides the necessary molecular spectroscopic information. The accuracy levels are determined through error analysis, highlighting the precision required for each molecule. The priority column indicates the order of importance or urgency, often based on scientific relevance or practical application. Each entry is linked to specific research, such as Yamada and Amano, indicating the primary sources for these data points.
**Radiative transfer calculation**

Brightness temperature:
- At the tangent height 1
- At the tangent height 2
- At the tangent height 3

**Doppler shift**

\[
 f_D = \left(1 + \frac{v_D}{c}\right)f
\]

\[
 v_D = v_{ISS} \cdot \cos \phi \cdot \frac{R_e + z_T}{R_c + z_{ISS}}, \quad \text{Re=Earth’s radius}
\]

**K to Watt/Hz**

\[
 P = kT \quad k: \text{boltzmann coefficient}
\]

**Optical loss**

**Standing wave**

**SSB filter**

**USB**

**LSB**

**Brightness temperature**:
- At the tangent height 1
- At the tangent height 2
- At the tangent height 3

**Cold sky**

**Hot load**

**Forward model development**

**SSB filter functions**

transmittance (+: USB, -: LSB): \[ t = \frac{1}{2} \{1 \pm \cos(\pi \left(\frac{2N + 1/2}{f_{L0}}, f_{fL}\right))\} \]

Power with transmittance:
\[ P(f_{fL}) = t(f_{fL})P_{in}(f_{fL}) \]

Power at frequency \( f_{fL} \):
\[ P_{out}(f_{fL}) = P(f_{L0} + f_{fL}) + P(f_{L0} - f_{fL}) \]
For AOS channel response function

\[ P_{\text{out}} = P_{\text{in}} + P_{\text{noise}} \]
\[ P_{\text{noise}} = \text{constant} \]

\[ f_{y2} = |f_{y1} - f_{L,02}| \]

Power with channel response function:
\[ P(f) = \sum_{i=1}^{i_{\text{max}}} P_{i} R(f, f_{i}) \]

Poiver for 1ch:
\[ P_{\text{ch}} = \int_{f_{\text{ch}, L}}^{f_{\text{ch}, H}} P(f) df \]

\[ T_{\text{obs}}(K) = \frac{P_{\text{obs}} - P_{\text{cold}}}{P_{\text{hot}} - P_{\text{cold}}} (T_{\text{hot}} - T_{\text{cold}}) + T_{\text{cold}} \]
\[ f = f_{D}/\left(1 + \frac{V_{D}}{c}\right) \]

USB, LSB loop

Tangent height, cold load, hot load loop

**Forward model development**
**Retrieval**

Optimal Estimation Method

- Linear least-squares method, allowing « a priori » knowledge to be taken into account
- Atmospheric parameters $x$ estimated by minimising $\chi^2$:

$$\chi^2 = \left[y - F(x, b)\right]^T \cdot S_y^{-1} \cdot \left[y - F(x, b)\right] + (x - x_0)^T \cdot S_{x_0}^{-1} \cdot (x - x_0)$$

- Weights: Measurement and « a priori » covariance matrices $S_y$ and $S_{x_0}$
- Diagnostics: Error covariance and averaging kernel matrices

$y$ : spectral measurements
$F(x, b)$ : forward model
$b$ : model parameters (spectroscopy, instrument)
$x_0$ : « a priori » parameter vector
Non-linear retrieval

*iterative Levenberg–Marquardt regularisation*

OEM with Levenberg–Marquardt iteration scheme:

\[
x_{i+1} = x_0 + (K_i^T S_y^{-1} K_i + S_{x_0}^{-1} + \gamma U)^{-1} \cdot \{K_i^T S_y^{-1} \cdot ([y - F(x_i, b)] + K_i [x_i - x_0]) + \gamma U [x_i - x_0]\}
\]

- **\( y \)**: spectral measurements
- **\( F(x,b) \)**: forward model
- **\( b \)**: model parameters (spectroscopy, instrument)
- **\( x_i, x_0 \)**: parameter and « a priori » parameter vector
- **\( S_{x_0}, S_y \)**: « a priori » and measurement covariance matrix
- **\( K = (\frac{\partial F}{\partial x}) \)**: weighting function matrix
- **\( \gamma \)**: Marquardt parameter. Convergence: \( \gamma \rightarrow 0 \)
- **\( U \)**: scaling matrix
- **\( S_b, K_b = (\frac{\partial F}{\partial b}) \)**: model parameter error covariance and weighting function matrices
Algorithm development for operational code

- Algorithms have been studied by NICT, Bremen university, and JAXA.

- In 2006, JAXA started the development of Operational Retrieval Code (ORC), and related algorithm studies

- Retrieval procedure based on:
  => Optimal Estimation Method
      look for a solution in the vicinity of an a priori value of the retrieved parameters
  => Levenberg–Marquardt iterative scheme for non linear inversion of strong lines

- Retrieved parameters:
  => Vertical distribution of the species VMR
  => Temperature distribution
  => Scan altitude offset + baseline parameters
Error estimations

Retrieval Errors: \( S \)

\[
S_{\text{total}} = S_{\text{statistic}} + S_{\text{null}} + S_{\text{model}}
\]

\[A = D K\] : averaging kernel matrix

\[S_{\text{statistic}} = D S_y D^T\] : statistical error

\[S_{\text{null}} = (A - U) S_{x_0} + (A - U)^T\] : smoothing error

\[S_{\text{model}} = (D K_b) S_b (D K_b)^T\] : model parameter error
Model parameter errors

Factors in model parameter errors
1. Calibration knowledge
2. Side Band knowledge
3. Antenna Pattern knowledge
4. Pointing knowledge
5. Spectroscopic parameter knowledge
6. AOS response function knowledge
Precision and accuracy

An example for $O_3$

1. Calibration knowledge
   (SW: Standing wave,
    GTV: time variation of the gain)
2. Side Band knowledge
   (SSB: SSB filter ratio)
3. Antenna Pattern knowledge
   (Antenna: Antenna pattern)
4. Pointing knowledge
   (THRE: Tangent height random error)
5. Spectroscopic parameter knowledge
   (PB: Pressure broadening error)
6. AOS response function knowledge
   (AOS: error from spectrometer)
**Examples for error estimations**

\[
S_{\text{total}} = S_{\text{statistic}} + S_{\text{null}} + S_{\text{model}}
\]

- \( O_3 \)
- \( \text{ClO} \)
- \( \text{HO}_2 \)
"Altitude scan off-set" can be retrieved.
→ improved to operational processing in JAXA.

"Pointing random error" is a major source of the error in O$_3$, HCl, and ClO retrieval.

What can we do for that?

**Tangent point retrieval and its error**

Error analysis
Tangent height retrieval

- Work still in progress but first results are promising.
- Tangent height retrieval improved the retrieval error of Ozone, HCl, significantly
**Ozone** *(mid-latitude scenario)*

Observation capability

<table>
<thead>
<tr>
<th>Observable Altitude region:</th>
<th>11 - 91km (tropopause 12km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Altitude resolution:</td>
<td>2.1km-6.2 km</td>
</tr>
</tbody>
</table>

**Band A**

**Band B**

**Band C**
BandC ClO (mid-latitude scenario)

Observable Altitude region:
24-63km

Altitude resolution:
3.5-8.1km
H₂O (mid-latitude scenario)

Observable Altitude region:  8 - 37km (tropopause 12km)
Altitude resolution:    2.4km-5.8 km

Band A

Band B

Band C
JEM/SMILES observation

**Observation capability**

* **Averaged profiles** (for example, zonal mean average/5km altitude resolution)