Impact of Molecular Absorption Spectroscopy Data on S5P Infrared Carbon Gas Concentration Retrievals — MADSICCC

Philipp Hochstaffl\textsuperscript{1}, Franz Schreier\textsuperscript{1}, Manfred Birk\textsuperscript{1}, André Butz\textsuperscript{2}

\textsuperscript{1}DLR — Remote Sensing Technology Institute
Oberpfaffenhofen, GERMANY

\textsuperscript{2}DLR — Institute of Atmospheric Physics
Oberpfaffenhofen, GERMANY

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Introduction — Motivation

- SWIR spectra of S5P/Tropomi contain information on CO, CH₄, . . .
- Various auxiliary data required for Level 1$\rightarrow$2 processing

How do molecular spectroscopy line data impact retrievals?
Molecular Spectroscopy Data

Lines in S5P-SWIR:

- CO
- CH$_4$
- H$_2$O

GEISA 2011: 518 13519 844
HITRAN 2012: 403 20578 1460
GEISA 2015: 518 14616 2921
HITRAN 2016: 310 15965 3169
SEOM–IAS : – 18218 –
Goals: Improve spectroscopic data in TROPOMI 2.3 \( \mu m \) region

Labs and Instruments:

- FTS measurements at DLR
  Bruker IFS 125HR, White-type multireflection cell
- CRDS (Cavity RingDown Spec.) measurements at LIPhy
  DFB laser based spectrometer 4248 – 4257 cm\(^{-1}\)

First results:

- \( \text{CH}_4 \): new line positions, intensities and additional line parameters in the range 4190–4340 cm\(^{-1}\)
- \( \text{CO} \): recommendation to use Hitran12
- \( \text{H}_2\text{O} \): Satisfactory agreement of FTS and CRDS intensities, major intensity differences to Hitran, good agreement with ab initio
- All: Residuals indicate narrowing and line mixing \( \rightarrow \) speed dependent Voigt with line mixing
Tools: BIRRA and RemoTeC

Beer InfraRed Retrieval Algorithm

- Separable least squares of molec. scale factors (and some aux. par.) to radiance
- Forward model: GARLIC
  Generic Atmospheric Radiation Lbl Infrared Code
- Originally developed for SCIA nadir CO, CH₄

RemoTeC

- “Full physics:” Retrieve gases and aerosols to account for light path modification
- Heritage: GOSAT (& OCO-2)
- Forward model: linearized vector rad. transfer
- Tikhonov regularization
Proposed Work

How do molecular spectroscopy line data impact retrievals?

- Update SEOM-IAS literature review
- Initial analysis performed on synthetic observations (see poster)
- Upgrade codes
  - BIRRA: S5P data ingestion, spectral response, refined line shape
  - RemoTeC: refined line shape
- S5P data processing: Comparison of total column retrievals using the SEOM-IAS database vs. Hitran, Geisa, ...
  - CO with BIRRA and CH$_4$ with RemoTeC
  - residual analysis
  - total columns and errors

→ Recommendations for further lab spectroscopy

References: see poster!