FTIR Technical Document

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Outline

- Work to date as appropriate to GRUAN
- Instrumentation
  - Data stream requirements
  - Auxiliary measurements
- Data Product Retrieval
  - Auxiliary data
  - Processing
  - Uncertainties

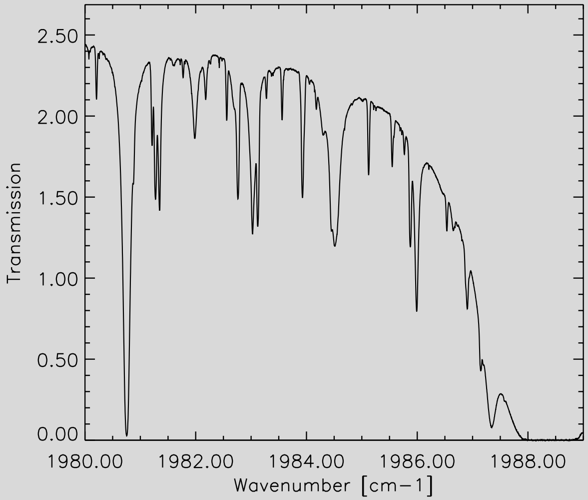
Work to Date

- Support TT5
- Boulder H_2O sonde / FTS retrievals
  - Coincident measurements 50, at MLO 30
- Discussed MUSICA project
  - H_2O / HDO focused IRWG sub-group
  - Central processing
- NORS project
  - Centralized post processing
  - Combined with model results
- Discussed:
  - Altitude sensitivity of some species (mostly H_2O)
  - Formal error analysis

Instrumentation

Typical Installation

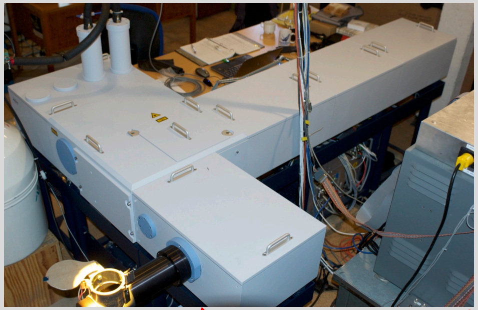
Custom 6" aperture, ephemeris + 1.3Mp camera dynamic solar tracker	$85,000
Bruker 125HR 250cm 700 – 15,000cm-1 FTIR	$400,000
LN2 Liquifier	$45,000
Auxiliary equipment	$20,000
Ability to resolve any terrestrial absorption feature in the mid – near IR at 2000+ SNR	***Priceless!***



Instrumentation

Communications & Controls

Bruker 125HR



TCP Data Server
- Live parameter distribution
- Remote access & control

Precision Solar Tracker

Weather Station

Sun Sensor

Windows Computer OPUS / Bruker Access

Linux Computer:
- Auxiliary data
- Weather / sun monitor
- Timing of spectral data collection
- Local & backup storage

LN2 Dewar: Daily Auto Fill InSb & MCT detectors

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

Daily download of spectral & auxiliary data, remote monitoring

Instrumentation

Species measured by high-resolution ground-based solar FTS in mid-IR, approx. DOFS from present analysis techniques.

Species	DOFS	Species	DOFS
H_2O	2 - 3	CH_4	2.5 - 3.5
CO_2	2 - 3.5	O_3	3 - 5
HF	2.5 - 3.5	C_2H_2	< 2
COF_2	< 2	C_2H_6	~ 2
HNO_3	2.5 - 4	OCS	3 - 4.5
NO_2	< 2.5	HCN	< 2.5
NO	< 2	SF_6	1*
N_2O	3 - 5	N_2	
CCl_2F_2	1*	CO	2.5 - 4
$CHClF_2$	1*	CCl_3F	1*
$ClONO_2$	1*	H_2CO	1
ClO	1	HCl	2.5 - 4

These 4 species referred to in BAMS 2016

GRUAN Justification document GCOS-112 specs:

Priority 1:
- H_2O at high vertical resolution (2-5%)

Priority 2:
O_3 and CH_4 at high vertical resolution and total column (3% & 2% resp.)

Priority 3:
CO_2 at high vertical resolution and total column (1%)

*limited by spectroscopy NDACC required product

Instrumentation

- Spectral Resolution
  - Do we want Total Column only or partial column data products?
  - Implications:
    - Instrument Selection / Design
    - Desired species
    - Cost
    - Acquisition time
    - Maintenance frequency / time / costs

Instrumentation

- Require
  - Scanner rate (laser fringe rate)
  - Optical band pass
  - Throughput
    - e.g. specifications on optical components
    - A level of radiometric calibration

- Solar Tracking Requirements:
  - Both active and ephemeris pointing
  - Solar disk pointing precision (~9arcsec)
  - Maximum variability in scan

Instrumentation

- Time based data acquisition e.g. Brault
  - Now default implementation in Bruker
    - But not Laser signal
  - Require both IR and Laser signal storage
  - Require DC recording
    - Including data rate, numerical precision
    - Source fluctuation correction (IR)
    - Modulation stability (laser)
  - Define electrical band-pass filtering
    - e.g. pre-amps
  - Dual channel (or wide band) recording
    - Reference O_2 band

Instrumentation

Effect of Spectral Resolution

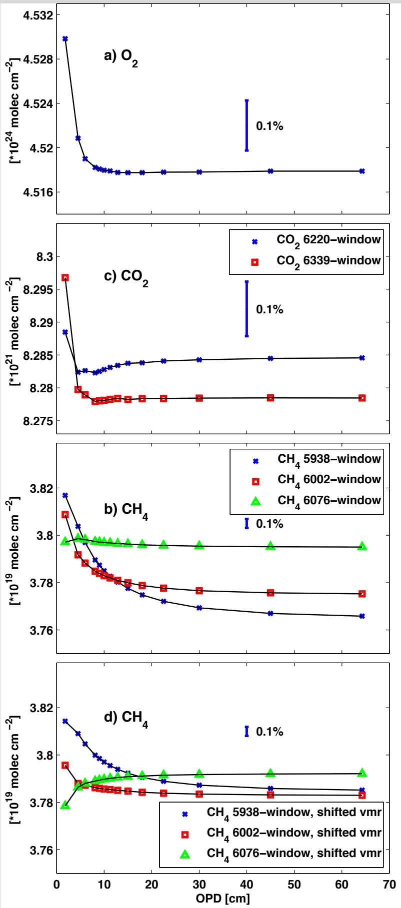


Fig. 10. Retrieved O_2, CO_2 and CH_4 total columns from the IFS 125 HR, by truncating the interferograms to different optical path differences. For CO_2 and CH_4 the different retrieval windows are shown. For CH_4 the initial a-priori profile has been shifted vertically by −4 km. The shown bars give a percentage scale.

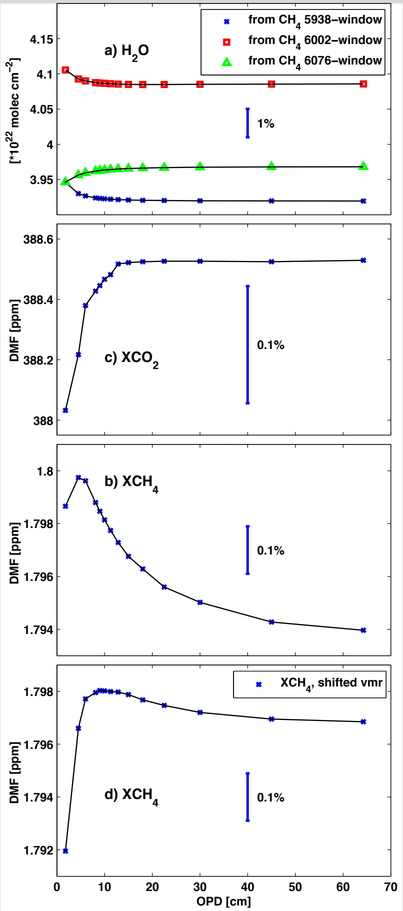


Fig. 11. Retrieved H_2O, XCO_2 and XCH_4 from the IFS 125 HR, H_2O is taken from the different retrieval windows of CH_4. For XCH_4 the initial a-priori profile has been shifted vertically by −4 km. The shown bars give a percentage scale.

- Each plots shows the variation in retrieved data as a function of increasing the OPD (increasing the spectral resolution).
- Left are total column [molec/cm^2].
- Right are dry air mole fraction [mean VMR]
- For all species / spectral regions tested there is significant change 0 to 5 or 10 cm.
- Accuracy limitations are prevalent with low resolution though not so with precision
- For total columns only 20cm may be sufficient

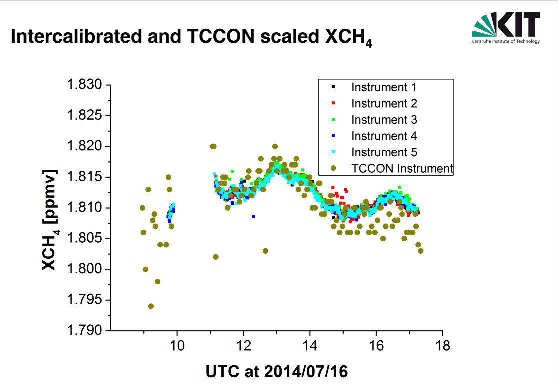
Remote sensing of CO_2 and CH_4 using solar absorption spectrometry with a low resolution spectrometer. , C. Petri et. al., Atm. Meas. Tech, 5(7):1627–1635, 2012.

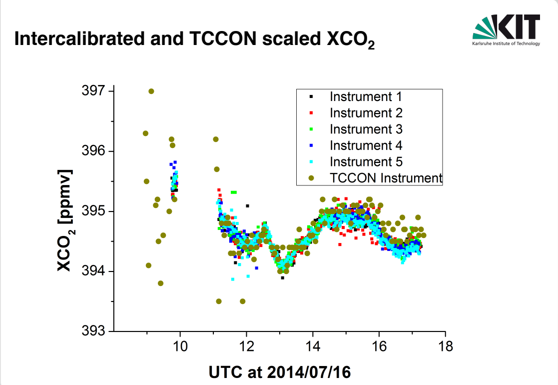
Instrumentation

Low Resolution

Low resolution Bruker EM-27Sun 0.5cm-1 + solar tracker

Compare xCO_2 & xCH_4 vs. a TCCON standard instrument
Calibration factor vs WMO: 0.9951





Above: KIT team at NCAR Foothills comparisons March 2015

- Still commercial ‘black box’
- Long term stability (multi year) not defined yet
- ILS & radiometric calibration issues
- ILS issues still convolved with interfering species

From Matthias Frey, KIT

Instrumentation

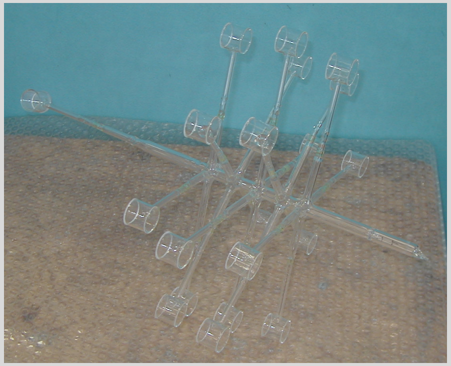
Moderate Resolution

Miniature Pointing Interferometer

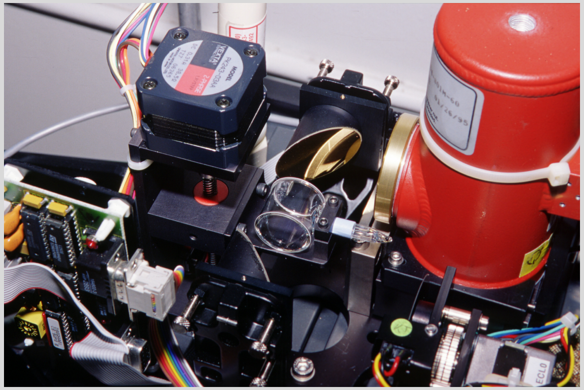
- Single moving mechanism (e.g. Bruker EM27, Bomem, ACE-FTS), but
- 20cm OPD / Resolution 0.05 cm^{-1} nominal
- Weather tight optical bench & electronics mounted on 2 axis motorized stage and pointed directly to sun.
- 3cm optical beam, corner cube reflectors
- Optical bench approx 15 x 15 x 30 cm
- Full mid to near-IR bandwidth 700 – 8000cm^{-1}
- Capture O_2 B band
- ZnSe beamsplitter (500-20,000 cm^{-1})
- DLaTGS or TE cooled MCT detector (no LN_2)
- TCP control & data access.

Instrumentation

Calibration Cell measurements



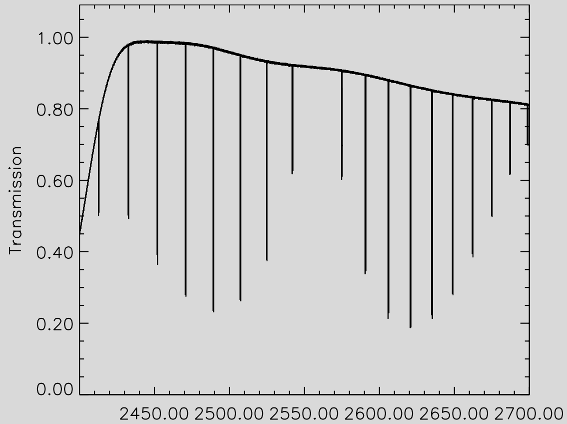
Manifold for producing 20 HBr (N2O) cells at common pressure.

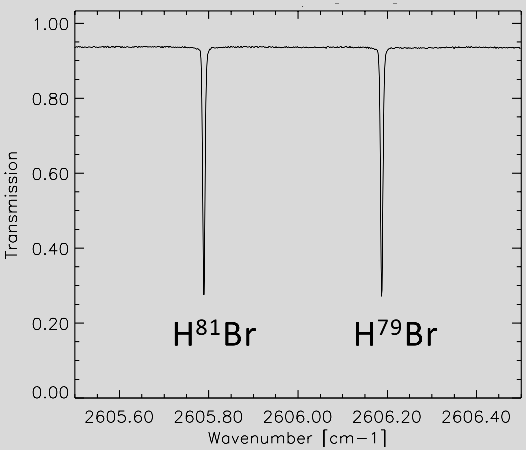


HBr cell mounted on motorized stage in Bruker 120M

- Line widths of absorption features are less then instrument response -> The ILS is analogous to a response to a δ-function.
- NDACC: HBr at 2mb , N_2O at 1mb in 2cm cell
- TCCON: HCl at 5mb in 10cm cell
- Other possible species OCS
- HBr can be measured without interference in solar spectra

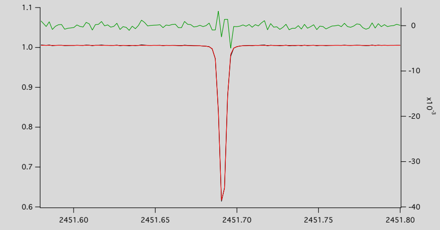
Instrumentation



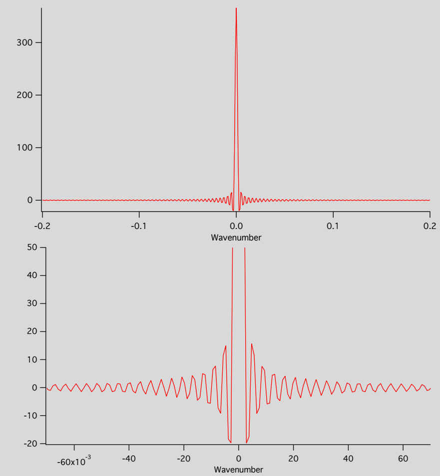


Retrieval of ILS at 4μm with HBr

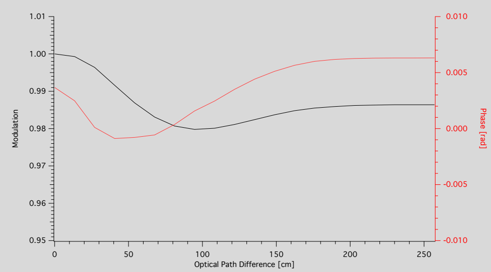
MLO ILS measurements with Cell #20 64 scans / SNR >2000



1 of 14 fits to HBr features



ILS fwhm = 0.0027cm^{-1}



Modulation Eff. And Phase from Linefit 11

To Maintain Reference Standards

- Accumulate calibrated spectra & interferograms
- Monitor instrument spectral and radiometic response over time
- Acquire spectra each e.g. day using internal source
- Acquire spectra e.g. day:time using sun
- Spectra & retrieved ILS comparable for all stations
- Retrieved ILS can be applied in forward model

Instrumentation

- Commit to specific species,
- Commit to product:
  - Column / profile e.g. Required DOFS,
- Define instrumentation
  - Spectral resolution,
  - Bandwidth,
  - O_2 channel,
- Remove hidden processes,
  - Bruker laser signal and initial processing.

Data Product Retrieval

- Transform of interferograms
  - Source intensity corrections
  - Detector non-linearity corrections
- QA/QC on spectra
  - Zero levels, phase, SNR, low frequency noise
- Preprocess
  - Acquire & process auxiliary retrieval input components
- Stepwise retrieval of target gases
  - Non-linear OE retrieval
  - Uncertainty estimates
- QA/QC on retrieved data products
  - Redundant measurements
  - Daily cell measurements

Data Product Retrieval

Retrieval Example

SFIT4:V0.9.4.1:20130708 RUNTIME:20131008-21:57:22

Fit : 1 06/23/2011 16:24:11UT Z:37.261 A:284.29 D:0101.7 R:0.0035 P:BX F:01.9139mr

IRET	GAS_NAME	IFPRF	APR_COLUMN	RET_COLUMN
1	CO2	T	6.58781E+21	6.89599E+21
2	O13CO	F	6.58781E+21	6.92287E+21
3	CO18O	F	6.58781E+21	7.44734E+21
4	HDO	F	1.38899E+23	4.39655E+22
5	H2O	F	1.38899E+23	5.49452E+22
6	H2180	F	1.38899E+23	6.44238E+22

IBAND	NUSTART	NUSTOP	SPACE	NPTSB	PMAX	FOVDIA	MEAN_SNR	NSCAN
1	4872.00000	4888.00000	0.002500000	6401	100.00	1.914000	94.506532	1

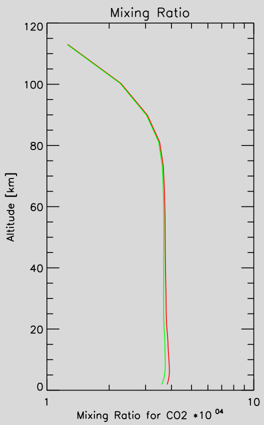
JSCAN	INIT_SNR	CALC_SNR
1	164.703220	94.506532

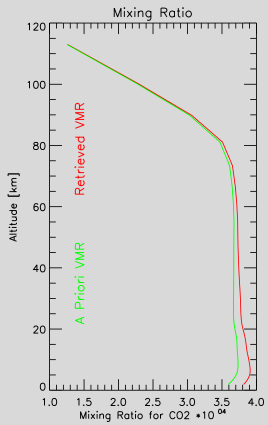
FITRMS	CHI_2_Y	DOFS_ALL	DOFS_TRG	DOFS_TPR	ITER	MAX_ITER	CONVERGED	DIVWARN
1.058045	3.036775	17.516	1.122	0.000	20	21	T	F

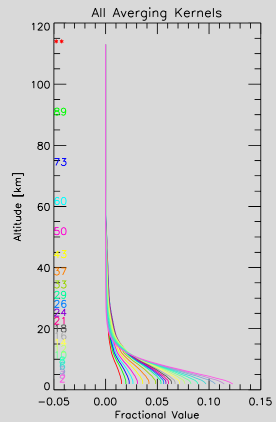
Retrieval Example $^{12}CO_2$ & $^{13}CO_2$

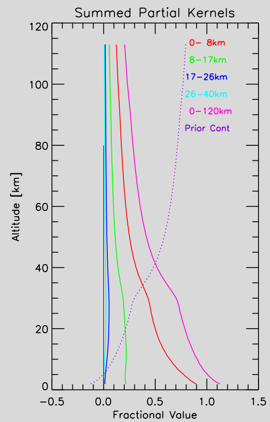
+ $CO^{18}O$, $H_2{}^{18}O$ & HDO

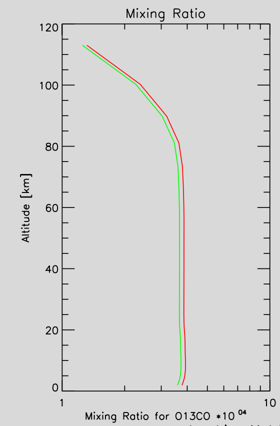
Boulder 23 Jun 2011

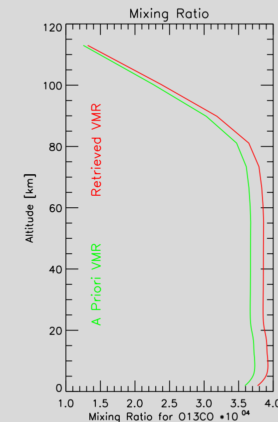


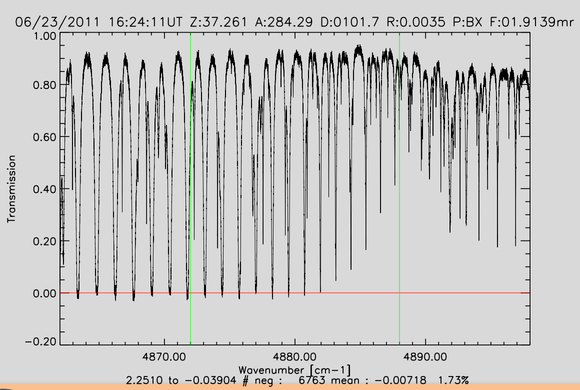


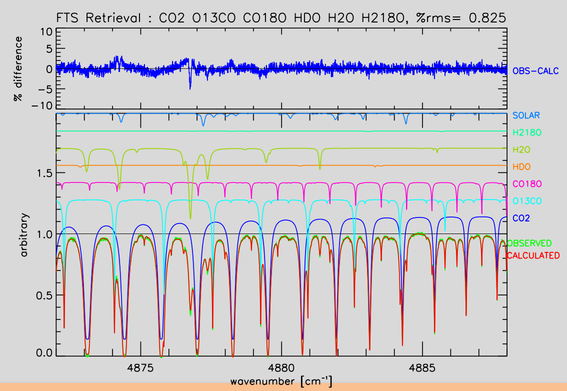


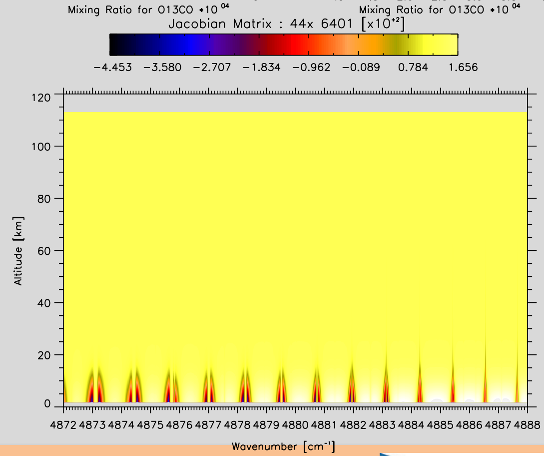












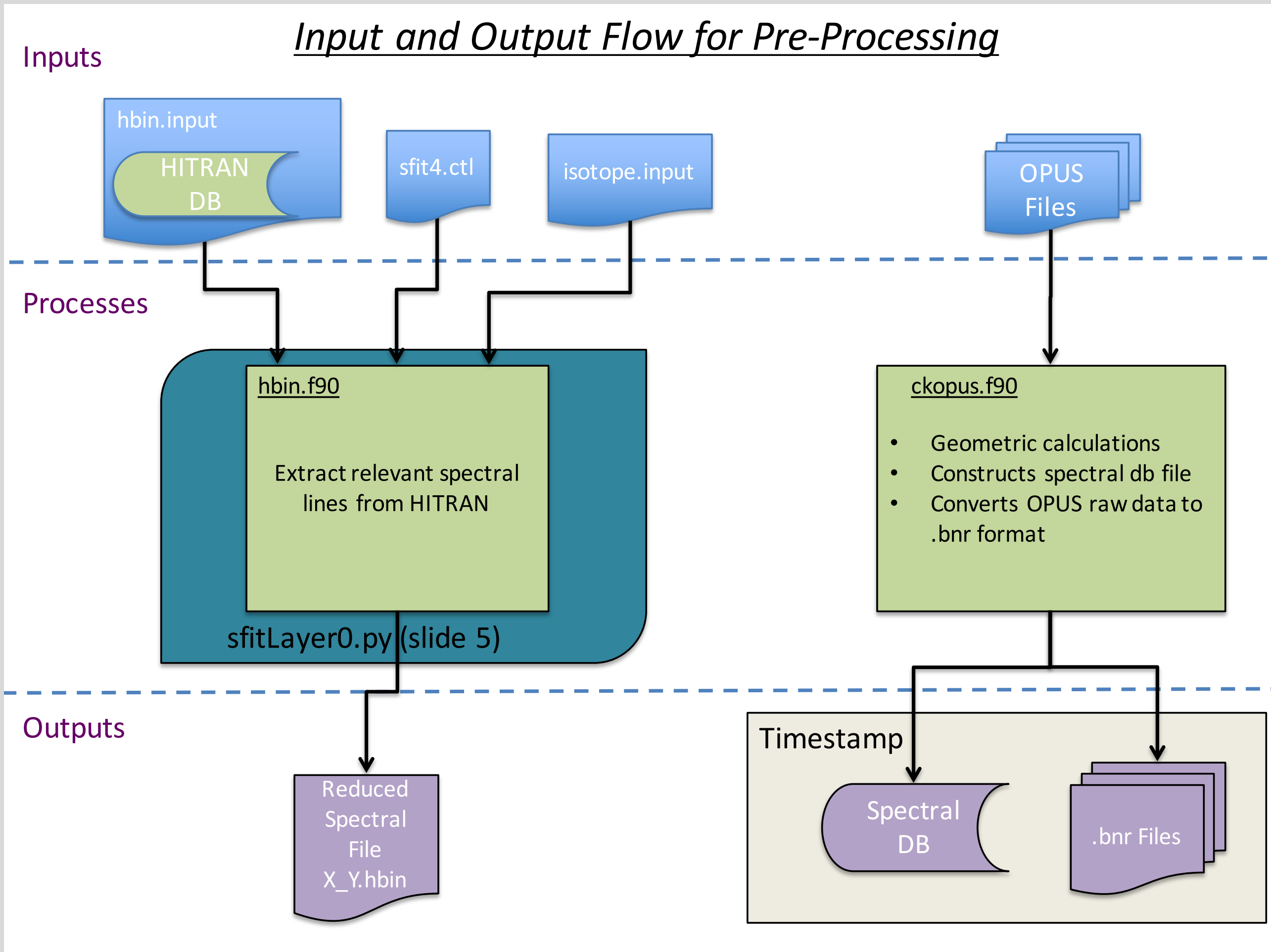
Data Product Retrieval

Auxiliary data required for consistent retrieval from globally diverse stations

- Consistent chemical a-priori profiles:
  - For target & interfering species, (NDACC:WACCM)
  - Perhaps constant, or best estimate on some time scale,
- Best estimate p-T profiles (NCEP, sonde),
- Spectroscopic data (e.g. HITRAN),
- Consistent retrieval grid,
- Precision temperature & pressure at observation location.

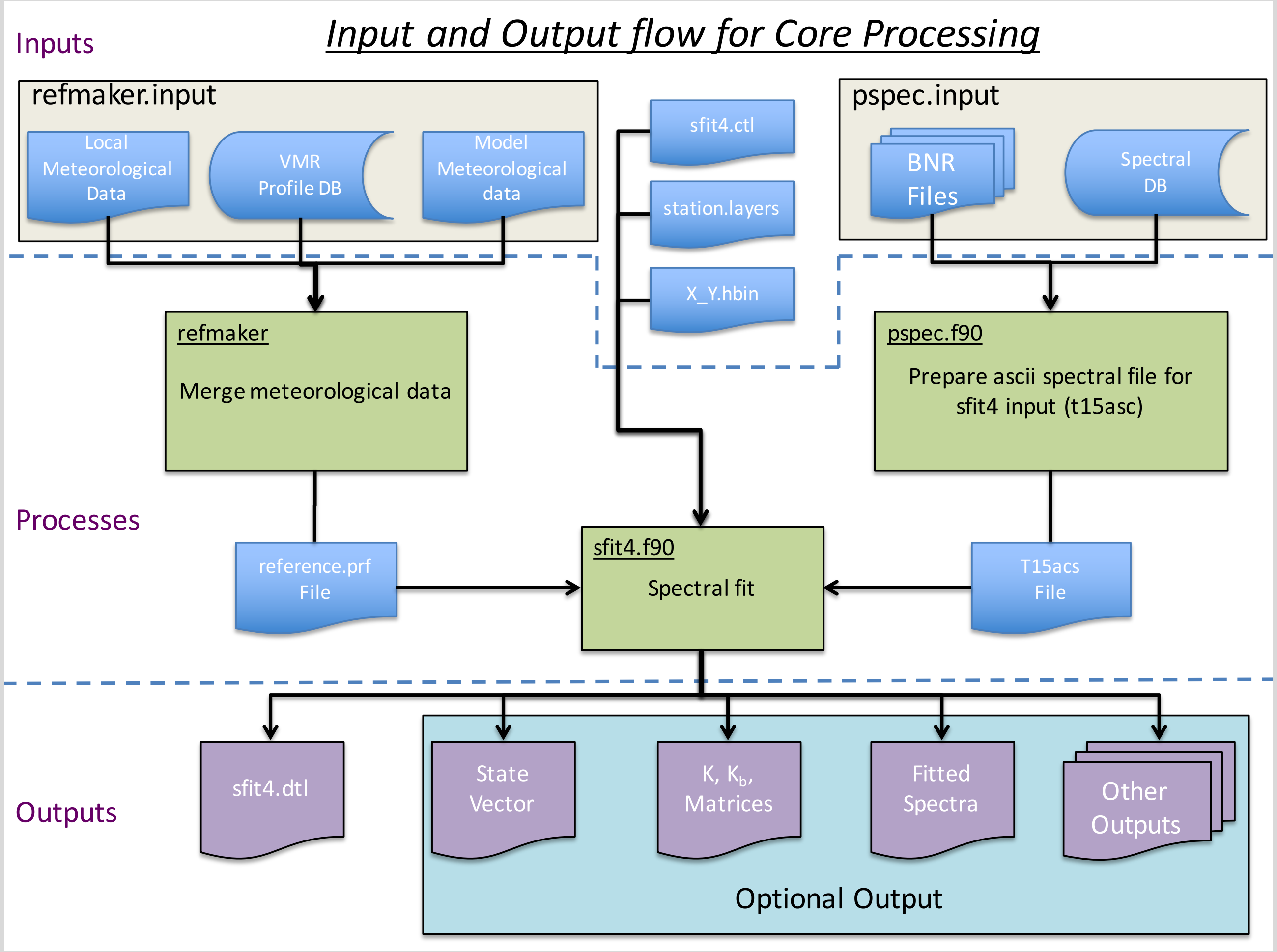
Data Product Retrieval

Pre-Processing

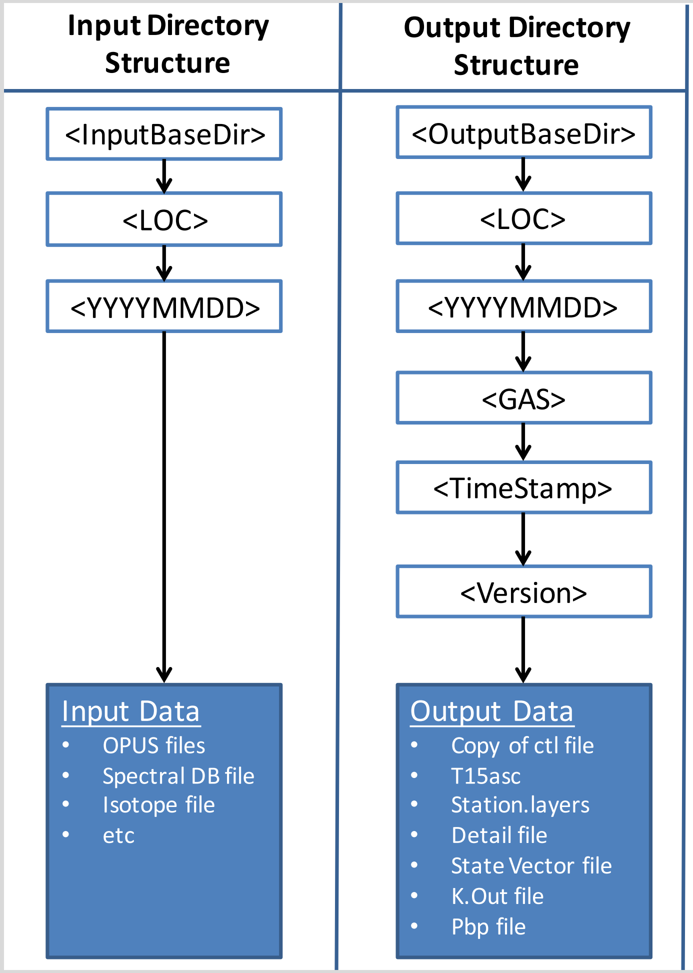


Data Product Retrieval

Processing Overview



Data Product Retrieval



- <InputBaseDir> : Base directory for input file structure
- <OutputBaseDir> : Base directory for output file structure (can be same as <InputBaseDir>
- <LOC> : Three letter site location abbreviation
- <YYYYMMDD> : Year, month, day of observation
- <GAS> : Primary gas of interest for retrieval
- <TimeStamp> : UTC time stamp of observation HHMMSS.SS
- <Version> : User defined description of ctl file used for processing

Data Product Retrieval Error Estimation

Instrumental / measurement / forward model parameters

- Background slope
- Background curvature
- Differential wavenumber shift
- Single wavenumber shift
- Independent wavenumber shift
- Empirical apodization function
- Empirical phase function
- Solar line shift
- Solar line strength
- Phase error
- Zero level offset
- Interfering species
- Channel parameters
- Field of View

- Target / Retrieved gas absorption line(s) *intensity*
- Target / Retrieved gas absorption line(s) *air broadened line half-width*
- Target / Retrieved gas absorption line(s) *temperature dependence*
- Other possible line parameters:
  - Self broadening
  - Lower state energy
  - Pressure shift
  - Galatry Beta
  - Line mixing parameters
  - S-DV parameters
- Solar pointing
- Temperature profile

Systematic & Random components calculated separately

Data Product Retrieval

- The sensitivity of X on a given b_i is minimized by early choices in the retrieval process (e.g. spectral region).

- The best estimate of S_{bi} may be
  - More or less obvious!,
  - Needs to be physically based,
  - May require sensitivity testing to determine,
  - Also needs to be 'homogeneous' across all sites.

- Error estimates are calculated for each level of each profile & column

- Error estimates can vary widely by species, station

Measurement Scheduling

- These are clear sky measurements,
- Moderate resolution data ~10sec,
- High resolution ~200sec,
- Data can be recorded at all clear sky solar zenith angles,
- Lunar measurements are much higher noise…
- Correlative measurements (redundancy)
  - Aircraft profiles
  - Side-by-side with multiple instruments

Data Management

- Raw streams for atmospheric & calibration delivered to Central Data Processing Center (CDPC)

- Transforms & corrections performed at CDPC,
- Retrievals (possibly) with sonde H_2O as apriori,
- Certainly with local z-p-T measured profiles,
- NRT processing dependent on a-priori availability,
- Software packages exist for retrieval and data flow,
- All retrieval intermediates should be archived – included in QA/QC e.g. drift analysis.

Summary

- FTIR Technical Document is in development
- Technique and processing is mature,
- Raw data QA/QC framework exists, detailed implementation plan and standards required,
- Software packages exist for retrieval and large dataset processing
  - detailed parameter selection required,
- Uncertainty estimate framework exists,
- Plan for redundancy TBD,
- Decisions required:
  - Given profile requirements do we target total column only for solar viewing IR trace gas measurements?
  - A-priori data sources

End