**Time Recording and Scan Properties in OPUS-run FTIR 120 HR measurements**

The purpose of this report is to detail the recording of FTIR measurements that will be useful in designing SFIT4, the new data processing program. The data from our FTIR are used to determine atmospheric gas concentrations and the precision of these measurements is important to understanding the composition of the atmosphere and how it is changing. Hence, it is critical to understand the input from OPUS to optimize the accuracy of these measurements.

This report will examine how OPUS records time during a measurement, the duration and other properties of scans, and determine the optimum time to measure the solar zenith angle for a certain measurement.

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1. ***Time-Stamp recording***

First we must determine at what point in a scan the timestamp is recorded by OPUS.

Observational times were recorded at scan start and zero-path difference (ZPD) and then compared with time-stamps recorded by the program OPUS. It is of importance to note that the clock is synched with NIST and hence accurate to detecting the small changes in solar zenith angle and air mass necessary for these measurements.

Table 1: Observed data is from the clock and OPUS data are IFGM times

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Scan type | Clock Start | IFGM Forward | IFGM Backward | Clock time at ZPD |
| 1 Forward | 6:49:45 | 6:49:55 |  | 6:49:55 |
| 1 Forward +1 Backward | 6:53:30 | 6:53:42 (ZPD of forward) | 6:53:46 (MPD of backward) | 6:53:42 |
| 2 Forward+ 2 Backward | 7:08:30 | 7:08:40 | 7:08:45 | 7:08:41 |

From these data, we can see that the times recorded by OPUS correspond to ZPD for the forward scans and maximum path difference (MPD) for backward scans.

For the forward+backward scan, the difference between the ZPD of the forward scan and the maximum path difference (MPD) is 4 seconds. This observational data is in agreement with the scan duration of 3.7 seconds recorded by OPUS.

The scan duration, when calculated from the scan resolution and velocity, is also in accordance with the OPUS-recorded duration.

Duration= MPD/Optical velocity=(1/Resolution)(velocity/15798)

Resolution is expressed in wavenumbers (cm-1), velocity is in Hz, and 15798 is the laser frequency, also expressed in wavenumbers. Hence for this investigation, done with .1 resolution and 40kHz velocity:

Duration= (.1\*15978)/40,000= 3.9 seconds

Though there is a slight difference between the OPUS-recorded duration and the calculated one, most likely caused by a small scanner oscillation before ZPD, these measurements show that the observed data match up with the time stamps recorded by OPUS.

**Calculating Expected Scan Time**

In this report, we define the term “scan time” as the time required by the FTIR to complete one *forward-only* scan with a fast return (velocity=80kHz). From the parameters of the FTIR scan, we can calculate what the scan duration should be given the resolution, phase resolution, velocity, and laser wavenumber.

The “phase time”, or theoretical time a scan should take, can be expressed as:

τ = γ\*τLASER ( + ) ( )

Where τ is the phase time,τLASER=15,798 cm-1 , the resolution is set at .01 cm-1 , the phase resolution is set at 4 (or sometimes 32) cm-1, and the velocity is nominally 40 kHz. The quantity γ is a ratio determined by Bruker and is equal to .9 for our instrument. Using this formula, we can generate expected scan times and compare those with actual times recorded manually or by OPUS to gain further insight into how OPUS records time and any discrepancies that exist in various scenarios.

Table 4: expected scan times for different resolution/phase resolution pairs assuming a constant velocity of 40 kHz. Resolution values in are on the left and phase resolutions run across the top.

|  |  |  |  |
| --- | --- | --- | --- |
|  | 4 | 8 | 32 |
| .01 | 35.63 s | 35.59 s | 35.56 s |
| .1 | 3.64 s | 3.60s | 3.57 s |

**Discrepancies between calculated and OPUS-recorded durations**

|  |  |  |
| --- | --- | --- |
| Scan Resolution (cm-1) | OPUS duration (seconds) | Calculated duration (seconds) |
| .01 | 39 | 36.4 |
| .05 | 7.9 | 7.28 |
| .1 | 3.9 | 3.64 |

These discrepancies exist but are not significant enough to require incorporation into the SFIT 4 program.

1. ***Time-stamping investigations—Variations on normal scans***

**Scan with lower velocity (10kHz)**

Table 5: Scan properties at 10 kHz

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Scan Type | Instrument Block’s # of scans | Acquisition Block’s # of scans | Instrument Block’s # of Good Fwd scans | Instrument Window’s # of Good Bkwd scans | Instrument Scan time |
| Forward | 2 | 4 | 2 | 0 | 46.07 s |
| Backward | 2 | 4 | 0 | 2 | 46.075 s |

Table 6: Time data for scan with velocity 10 kHz

|  |  |  |  |
| --- | --- | --- | --- |
| Clock Start | IFGM Forward | IFGM Backward | Clock time at ZPD |
| 7:41:50 | 7:42:19 | 7:42:09 | 7:42:25 |

**Scans with a Fast Return**

This section looks at scan sets with a forward scan at 40 kHz and a fast return backward scan at 80kHz. For the fast return, the time between laser wavelengths, τau, is 12.5 μs.

1) 4 scan sets

Table 7: Scan properties for fast return investigation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Peak Location | Instrument Block’s # of scans | Acquisition Block’s # of scans | Resolution | Instrument Scan time |
| 709 cm-1 | 8 | 8 | .01 cm-1 | 416.015 s |

To find the time elapsed for one, forward scan:

τSCAN=MPD/vOPTICAL=15798/(.01\*40000)=39.5 seconds

We use the same formula to obtain the time required for the fast return:

τRETURN=15798/(.01\*80000)=19.75 seconds

Hence:

τTOTAL=8 forward scans\* τSCAN+7 backward scans\* τRETURN=454.2 seconds

However, there is a 38 second or so time discrepancy between this calculated result and the one recorded in the OPUS instrument block.

2) 2 Scan sets at .1 resolution

2\*3.9≅8+1/2\*4= 10 seconds (duration also equals 10 seconds in the OPUS file)

3) 8 scan sets at .1 resolution

8\*3.9 +7\*3.9/2= 44.9seconds (duration equals 48 seconds in the file)

4) 8 scan sets at .05 resolution

8\*7.9+&\*2.95= 90.85 seconds (duration equals 88.89 seconds in the file)

5) 8 scan sets with resolution=.01, phase resolution=4

τ1= .9\*τLASER(1/Resolution+1/Phase Resolution)\*1/Velocity= 35.63 seconds

τRETURN=.9\* τLASER(1/Resolution)\*1/Velocity=17.78 seconds

Hence

ΤALL= 8\* τ1+7\* τRETURN= 409 seconds

**Time Stamping when the Digital Filters are turned off**

It is also important to determine whether the presence of a digital filter, which is present during most FTIR measurements, affects the time stamp. We took data for a scan with no digital filters. The phase resolution was set at 4 cm-1(14,218 points) for this scan, whose properties are shown below along with the time data.

Table 7: Time data for a scan taken without digital filters in place

|  |  |  |  |
| --- | --- | --- | --- |
| Clock Start | IFGM Forward | IFGM Backward | Clock time at ZPD |
| 7:50:00 | 7:57:19 | 7:57:35 | 7:57:20 |

***3. General Properties of Scans***

As we come to understand the time stamping properties of OPUS, it is good to become familiar with the way OPUS saves the data acquired by the FTIR and categorizes the scans that generated those data.

Table 2: Scan Properties as recorded by OPUS

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Scan Type | Instrument Block’s # of scans | Acquisition Block’s # of scans | Instrument Block’s # of Good Fwd scans | Instrument Window’s # of Good Bkwd scans | Instrument Scan time |
| Forward | 2 | 4 | 2 | 0 | 46.009 s |
| Backward | 2 | 4 | 0 | 2 | 46.01 s |

Table 3: Phase Resolution properties

|  |  |  |
| --- | --- | --- |
| Phase Resolution | Number of Points in interferogram | Phase Optical Path Difference (cm) |
| 4 | 14218 | .25 |
| 40 | 1421 | .025 |

From the fundamental properties of a scan, we can also determine the point spacing of the interferogram, Δν, using the following formula:

Δx=

Where Δx is the movable mirror’s change in position and N is the number of points in the interferogram. These properties are both ultimately derived from the phase resolution and resolution of a given scan.

**Calculating the Peak Location of Scans (ZPD)**

To find the location of ZPD for a scan, we use the optical properties of the lasers as well as the input phase resolution. The location of ZPD is defined as its distance from the optical switch of the FTIR. The following result was also confirmed with manual measurement.

Peak Location (PKL) of Laser\*2= 79,707 waves/cm (zero times) and

79,707/4=19,927 waves

Given this and the laser wavenumber, 15798 cm-1, we can find the peak location (PKL) with respect to the optical switch.

PKL in cm=19927/15798=1.26 cm

**Calculation of and Importance of ZPD time**

Finding the exact air mass a beam of light goes through before entering the FTIR is important for obtaining accurate atmospheric gas concentrations. Hence, it is crucial to compute the solar zenith angle that most accurately represents the path of the rays that enter the FTIR during a measurement. Since solar zenith angle is a function of time, we need to use the average ZPD time during a measurement to process the data. The average ZPD time can be computed from the timestamps recorded by OPUS as well as the scan length. We define this time as the average elapsed time between the scanner being at ZPD in consecutive scans.

From investigating the FTIR and how OPUS records time during its measurements, we can define the average ZPD time mathematically as:

ΤAVG ZPD=(T1+T2+τSCAN)/2

where T1 and T2 are the time stamps recorded by OPUS on consecutive forward and backward scans.

**Conclusion**

With this information, we can better understand the FTIR measurement process and its relation to OPUS. Most importantly, we determined that OPUS puts a time stamp of a given forward scan at ZPD and at MPD for a backward scan. Hence we now can compute average ZPD time from the OPUS inputs and can incorporate this into the SFIT4 program to improve the accuracy of our atmospheric gas measurements.

**4. Specific Cases**

**4.1 ver 1.4 OPUS / 120HR AQP boards**

1995-2009 MLO

version 1.4 OPUS / 120HR AQP boards

timestamp for phase and emission blocks are different:

$ ckopus -SMLO -P h4582506.0

OPUS DAT & TIM strings:

EMIS: 25/08/1995 08:02:24

PHAS: 25/08/1995 07:59:57

here 147 seconds but often a little less and in opus2md hardcoded as 138s

Standard DU processing was to use phase and subtract 150s (288 id using EMIS block)

\*Assume here that even the earlier time (PHAS) is at the end of the measurement\*

(Then (maybe) the EMIS time is at end of file write?)

For this file:

$ ckopus -SMLO -b5 -C -U -pPHAS -t-150 h9582506.1

time one scan: 107.209516

time for fast return: 41.685159

time for down & back: 148.894676 (time between first & last ZPD's)

calculate duration: 256.104192 (2\*down + 1\*back)

duration (from file): 256.104192

final adjustment: -75.552662

Or

ckopus -SMLO -b6 -C -U -pPHAS h9582506.1

Option 6 does a similar calculation but assumes the PHAS timestamp is at the end of the last forward scan. With this option no fixed adjustment is needed.

ZPD time worksheet from test of version OPUS 1.41 on FL0 120HR 0 This should mimic the 1995-2009 MLO Bruker. Many XMP's from that time have PHAS - 4:22 in the OPUS header block. Defining the time difference between the PHAS time stamp and the start of the first ZPD as calculated/verified by this test.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | PC clock time from visual location of scanner | | | | |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  | dwn | bak | dwn2 | bak2 |  |  |  |  |  |
|  | zpd | end | zpd2 | end2 | zpd |  |  |  |  |
| time of day | 23:01:18 | 23:03:01 | 23:03:51 | 23:05:33 | 23:06:24 |  |  |  |  |
| time diff |  | 0:01:43 | 0:00:50 | 0:01:42 | 0:00:51 |  | From File |  |  |
| seconds diff |  | 103 | 50 | 102 | 51 |  |  |  |  |
| dwn+bak+dwn | |  |  | 255 |  |  | PHAS | 23:05:39 |  |
|  |  |  |  |  |  |  | EMIS | 23:08:05 |  |
|  |  |  |  |  |  |  | diff | 0:02:26 | 146.00 |
|  |  |  |  |  |  |  | DUR | 256.2 |  |
| time diff PHAS - ZPD | | 00:04:21 | 261.00 | (~ DUR) |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
| time diff EMIS - ZPD | | 00:06:47 | 407.00 |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
| time start to midpoint | | 77 |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
| PHAS time is the time after the last fwd ifgm data point is taken | | | | | |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
| mean ZPD time is PHAS - dwn - 77 | | | |  |  | -180 |  |  |  |
|  |  |  |  |  |  |  |  |  |  |

**4.2 Ver 7 OPUS (linux) 125HR**

MLO 125 - after August 2011

ckopus -SMLO -b3 -C s3ifml00.1

clock is UTC

xpms are 2 forward or 1f-1b

using –b4 or –b5 whether fwd or fwd/bkd is determined internally so we can use the same -b flag for any file.

**5. ckopus Readme file**

Readme for ckopus.c

Some caveats and possible causes for errors

velocity

for os/2 v3 of opus the velocity value in opus was the index to an array of velocity values in Hz

for 125 it is the floating point value in kHz

we have a simple check for the '.'

This works so far mat may fail with some other configuration

aperture

is read from a string to a float with units of mm

optical filter

is read as a 1 char string from a multi word string

this string is editable and may be different at any site!

on 2 filter wheel systems the combination of positions determines the designation

we have this for MLO but this needs to be changed for your site.

see function filterid() in ckopus.c

August 2013

Included a check for internally determining if a fwd only or fwd/bkd file for 125

siteflag must be 3 (fwd) or 4(fwd/bkd) but will be changed if the file is the other type

July 2013

added check for OPUS magic number

return codes

1 = cannot open file given

3 = opened file but not an OPUS file (incorrect magic #)

added time correction flags

0 - default no time correction

1 - empirical value given in -t time to block time

2 - for 2 file forward / backward scheme (OPUS v3.04 OS/2 ~1996) plus -t time

3 - forward only fast return plus -t time

4 - forward / backward one file (IFS125) plus -t time

5 - forward only fast return plus -t time (use scantime duration value)

6 - forward only fast return plus -t time (use scantime duration, file time is end of scan)

these are ways to adjust the the time that I am aware of, its likely not complete

I don't know if there is a document or map for conversions for all opus versions / IFS models

so this is a work in progress. You can view the error file for some details on the offset it

calculates

25 June 2013 V1.0 --- jwh

Ckopus has many useful features for looking at OPUS file contents, converting spectral

data blocks to other formats and acquiring pertinent data for a database. Type ckopus -?

for a list of features.

In particular it also calculates the solar position given the lat lon and time of measurement.

See the file constant.c (h) to add a new site to the built in sites for lat, lon, UTC offset etc.

The UTC offset can be applied (when the instrument is on local time see option -U) or not.

Time is a tricky issue with OPUS files. There is consensus that the time of ZPD should be used

for the calculation of the solar zenith angle. Deriving that time from the OPUS file write

timestamp or a time given in a data block is not so straight forward. For new instruments

it may be largely settled but for the older instruments and versions of OPUS going back

to V1.4 on OS/2 in the early 1990's it was not clear. Different groups worked out

procedures appropriate to their needs.

The current version of ckopus does not make any adjustments yet. So beware.

For early opus versions (MLO, OS/2, OPUS v1.4) it was found that the time in the PHAS block was

at zpd at about 2:18 earlier than the EMIS block. For later OPUS (TAB, OS/2, OPUS V3) all

blocks had the same time stamp (PHAS, SNGC, IFGM) and this held true for MLO 125HR. Hence it

defaults to the PHAS block. Other groups calculated the zpd time from the file write timestamp

FWD / BKD number of scans the resolution and scanner velocity. This relies on the file

write timestamp being preserved. This can be code in but as yet has not. I don't believe

these options are conclusive so other options may need to be included. Then as well some way of

choosing which to employ. It can be a combination of site and date.

If you have a calculation that you put in or wish to have put in let me know.

-Jim

jamesw@ucar.edu

usage:

printf( "usage: ckopus -wXXX -nXXX -aXXX -tNNN -s -Ssss -[S|L|B|P|R] -[R|F]ssss file1 file2 ...\n" );

printf( "where:\n" );

printf( " -v print the current version\n" );

printf( " -w is west longitude defaults to %.2lf [decimal degrees]\n",site.w\_lon );

printf( " -n is north latitude defaults to %.2lf [decimal degrees]\n", site.n\_lat );

printf( " -a is altitude defaults to %.2lf [meters]\n", site.altud );

printf( " -t is time offset defaults to %i [seconds]\n", site.sec\_offs );

printf( " -p use this block for time calculations [TRAN | SGN2 | IFG2 | EMIS | IFGM | PHAS | SNGC] ex. -pSNGC \n" );

printf( " -b Bruker time calculation flag\n" );

printf( " 0 - default no time correction\n" );

printf( " 1 - empirical value given in -t time to block time\n" );

printf( " 2 - for 2 file forward / backward scheme (OPUS v3.04 OS/2 ~1996) plus -t time\n" );

printf( " 3 - forward only fast return plus -t time\n" );

printf( " 4 - forward / backward one file (IFS125) plus -t time\n" );

printf( " 5 - forward only fast return plus -t time (use scantime duration value)\n" );

printf( " 6 - forward only fast return plus -t time (use scantime duration, file time is end of scan)\n" );

printf( " -u is UTC time offset defaults to %i [hours]\n", site.utc\_offs );

printf( " -U apply UTC time offset\n" );

printf( " -s swap bytes on opus read defaults to No Swap\n" );

printf( " -S set lat lon & alt for [TAB | FL0 | MLO | KPK | PKF | MSA | SGP | TMK]\n" );

printf( " -C short listing of file contents\n" );

printf( " -L long listing of file contents\n" );

printf( " -B list file blocks\n" );

printf( " -P list time stamps\n" );

printf( " -M make Linefit microwindow files\n" );

printf( " -R write 'C' bnr from type [TRAN | SGN2 | IFG2 | EMIS | IFGM | PHAS | SNGC] ex. -RSNGC \n" );

printf( " -F write FORTRAN bnr from type [TRAN | SGN2 | IFG2 | EMIS | IFGM | PHAS | SNGC] ex. -FEMIS \n" );

printf( " -T write T15asc file from type [TRAN | SGN2 | IFG2 | EMIS | IFGM | PHAS | SNGC] ex. -TEMIS \n" );

printf( " -D one line param list for database to stdout ex. -DEMIS\n" );

printf( " -H print database header to stdout\n" );