An intercomparison of solar MIR-FTS measurements of atmospheric gases between a Bruker 120HR and a Bruker 125HR at Lauder, New Zealand (45S)

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1. Summary

Bruker 125HR (NIWA006) MIR NDACC observations started at Lauder in November 2017, with the aim of replacing the aging Bruker 120HR (NIWA001). An instrument intercomparison was conducted from November 2017 to May 2018 with a total of 20 comparison days. Each instrument had a dedicated solar tracker and a full set of NDACC narrow-band filters. Overall, the 125HR has superior signal to noise characteristics (for similar acquisition settings) and half the spectra acquisition time of the 120HR. Comparison of total column abundances for the 10 NDACC species show they are in agreement, with mean differences less than the combined measurement random uncertainty however, measurement bias for $ClONO_2$ and C_2H_6 are greater than 5%. NIWA006 data are to be submitted to the NDACC database. Comparison of partial columns (and/or profiles) for all species incorporating robust uncertainty analysis is planned.

2. Motivation

The incumbent Bruker 120HR was installed at Lauder in October 2001. There had been an increase in random and systematic problems with the instrument over the past few years. For example the AQP card is not supported beyond Windows XP and a random exit aperture indexing error developed. A decision was made to continue the long term NDACC MIR observations with the Lauder 'TCCON' Bruker 125HR. An intercomparison between the two FTIRs was performed before possible failure of the 120HR. Such an intercomparison is critical for trace gas time series continuity, and compliance with NDACC observation procedures (Griffith, 2003, JTECH).

3. NDACC MIR obs on the Bruker 125HR.

The Lauder 125HR was installed at Lauder by John Robinson and Gregor Surawicz in August 2009. The instruments primary role was to perform routine NIR 'TCCON' measurements and provide back up NDACC MIR measurements in case of failure of the Lauder 120HR. The new 125HR was additionally equipped with InSb and HgCdTe detectors, and a paired KBr beam splitter. Sporadic MIR measurements were taken between 2009 and 2018 with a limited MIR narrow-band filter set. In 2018 the surplus Arrival Heights 120M NDACC MIR filter set (#1-6) was installed into the 125HR. The Lauder 120HR has a split filter #6, into filters #8 (750-1050cm^{-1}) and #7 (950-1250cm^{-1}). The 125HR filters #1, #2 & #3 have larger bandwidths, as seen in figure 1. Table 1 lists SNR calculations per filter, per instrument over a year of operation. Overall, the 125HR has better SNR except in a few circumstances where the 120HR acquisition settings cause higher SNR, e.g. filter #2.

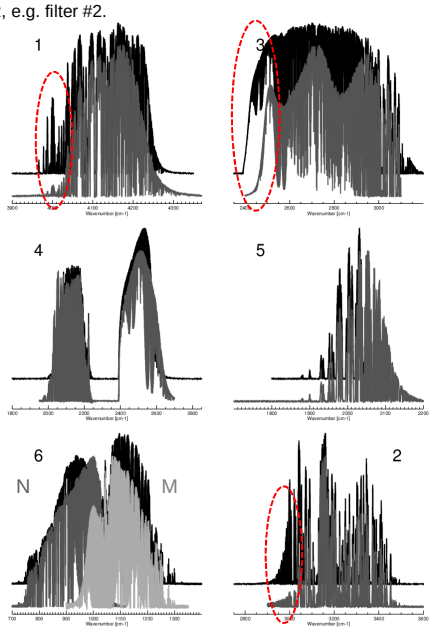

Figure 1. An example of typical spectra taken on each instrument with each NDACC filter (on 29/1/2018). Black = 125HR, Grey = 120HR. NDACC filter number for each spectra is displayed. 125HR spectra have been vertically offset to allow a better comparison.

NDACC Filter No.	Wavenumber range (cm^{-1})	SNR calculation window	SNR: 120HR 2017 Mean (σ) #obs	SNR: 125HR 2018 Mean (σ) #obs
1	3900 - 4300	4038.80 - 4038.90	485 (160) 649	764 (285) 645
3	2400 - 3100	2908.85 - 2909.00	609 (204) 815	620 (103) 660
4	1750 - 2800	2143.5 – 2143.63	677 (277) 771	1358 (242) 698
5	1800 - 2100	1985.19 – 1985.90	369 (152) 740	419 (173) 739
6	700 – 1350	844.5-845.4		182 (36) 763
8	750-1050	844.5-845.4	239(48)667	
7	950-1250	1157.01-1157.11	267(53)656	
2	2800 - 3500	3204.42 – 3204.64	3415 (1018) 656	1835 (377) 708

Table 1. SNR of spectra taken with NDACC filters used in the 120HR and 125HR. The mean SNR (along with 1-σ s.d. and number of observations) of each filter over one year are listed. The selected SNR calculation-year differs as there was not an entire year over which both instruments operated in parallel.

4. Intercomparison measurements

Both FTIR systems had their own dedicated solar tracker of similar type (NIWA360 tracker, pointing accuracy +/-0.02 deg). Comparison measurements were taken in parallel. There were 20 comparison days spanning 6 months (November 2017 to May 2018). A total of 797 and 407 spectra were taken for the Lauder 125HR and 120HR respectively. The 125HR acquired double the amount of 120HR observations due to faster FFT computations. Both instruments operated under vacuum (<5hPa), and with similar acquisition (XPM) settings. Gains and apertures were set per instrument to maximise signal level. All measurements were taken at a spectral resolution of 0.0035cm^{-1} (except for 120HR filter #2, 0.007cm^{-1}) ILS and ILS stability were checked monthly (via HBr and N_2O cell spectra analysis). Figure 2 shows typical ILS for each instrument. Figure 3 displays ILS modulation efficiency and phase error for each instrument, from monthly cell tests and analysis over the 6 month comparison period. Both instruments exhibit stable ILS, low phase error and are comparable.

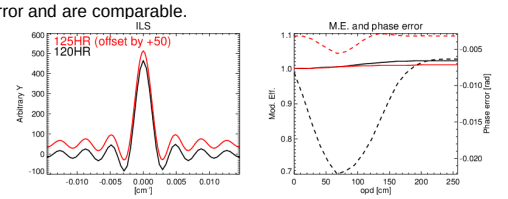

Figure 2. ILSs for both instruments from Linefit12 analysis of HBr Cell#21 spectra taken on the 6th and 18th September 2017, just prior to intercomparison. Solid lines in the second panel are the retrieved modulation efficiencies (M.E.). The dashed lines are the phase error.

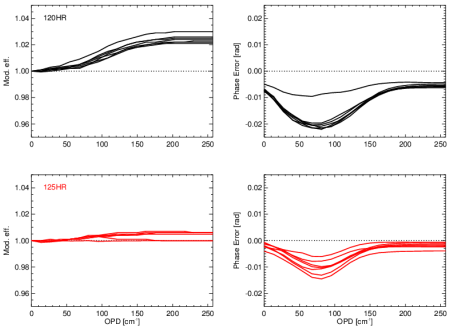

Figure 3. ILSs and phase errors (top two panels = 120HR, bottom two panels = 125HR) derived from monthly cell tests (7 per instrument) and analysis during the intercomparison period.

5. Retrievals

Trace gas retrievals are performed using SFIT4_v0944 for all 10 NDACC species (HF, HCl, HCN, $ClONO_2$, O_3, HNO_3, CO, C_2H_6, CH_4 & N_2O) using NDACC-compliant retrieval strategies with SNR (Se) optimised per instrument and species. In both cases the same retrieval specifications (linelist, MWs, PT profiles etc.) are used. See Table S1 for parameter retrieval details. An ideal ILS (and phase error of zero) is used in the 120HR &125HR spectra analysis. Total column (TC) retrievals spanning the intercomparison period for both instruments are shown in figure 4.

6. Intercomparison analysis and results

Intercomparison methodology is similar to that in used Batchelor, 2009, JTECH. For each species, measurements were compared on a day to day basis.

For each species, the TC mean-weighted bias for the 125HR (with respect to the 120HR retrievals) for each day of comparison measurements are given, (section S2). A summary is listed in Table 2. For all species, comparison of species total column amounts are shown to be in agreement within the combined measurement uncertainty over a large range of atmospheric conditions. Biases in $ClONO_2$ and C_2H_6 are greater than 5%, the causes need to be found and addressed. The calculated biases are similar in magnitude with other NDACC MIR FTIR intercomparison campaigns: Griffith (2003), Batchelor (2009), Paton-Walsh (2008, JTECH), Goldman (1999, JGR) and Smale (2017, IRWG-Paris, poster).

Species	Comparison days	Total number of comparison spectra (120HR, 125HR)	Bias: Mean TC Diff(%)	Measurement uncertainty: Random component (%) (120HR, 125HR)
O_3	9	41, 105	-1.19	1.6,1.6
HNO_3	5	25, 58	2.19	2.0, 2.0
HF	9	61, 115	0.06	1.3, 1.3
HCl	8	65, 107	1.19	1.5, 1.7
$ClONO_2$	2	10, 27	-8.01	19.6, 5.96
N_2O	7	60, 95	0.16	0.8, 0.8
CH_4	8	68, 110	0.46	1.2, 1.2
CO	7	54, 98	0.22	1.4, 1.3
C_2H_6	9	57, 96	8.05	10.0, 8.5
HCN	9	64, 99	-0.93	4.3, 5.3

Table 2. Summary of Mean TC Diff(%) for all 10 species. The total number of comparison days and number of spectra taken per instrument are also listed. The indicative random component of the measurement uncertainty, per instrument, per species is also tabulated.

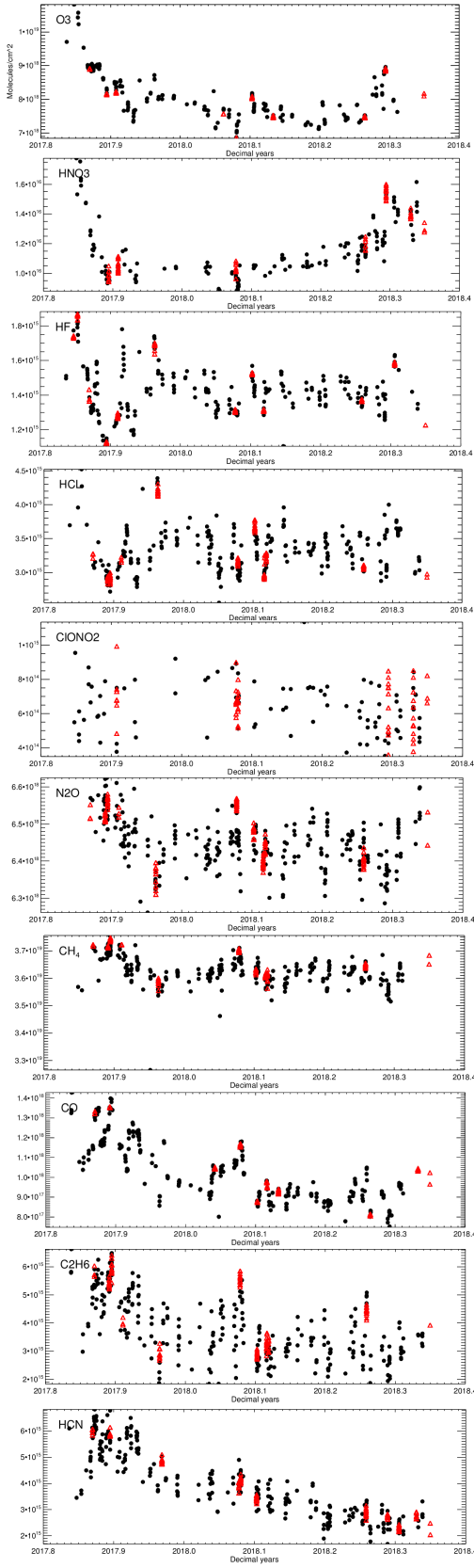

Figure 4. Total column time series for the 10 NDACC species over the comparison period Nov 2017 – May 2018. Black = 120HR, Red = 125HR. There were MIR and NIR observation time sharing on the 125HR during the intercomparison. NIR obs took priority, hence the lack of MIR obs.

7. Further work

- Perform partial column and/or profile comparisons.
- Incorporate sfit4 uncertainty analysis into comparison statistics.
- Submit NIWA006 trace gas retrievals to the NDACC database.

Acknowledgments

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Supplementary material: An intercomparison of solar MIR-FTS measurements of atmospheric gases between a Bruker 120HR and a Bruker 125HR at Lauder, New Zealand (45S)

S1. Summary of the retrieval parameters

A description of species retrieval parameters are given in table S1. For each instrument the ILS is assumed ideal (and phase error is zero). All retrievals are performed with SFIT4_v0944 and use daily NCEP pressure & temperature profiles.

Table S1 foot notes:

A: WACCM refb2.1 monthly climatology was used to keep consistency with the retrieval strategy used in Vigouroux, C., et al.: Trends of ozone total columns and vertical distribution from FTIR observations at eight NDACC stations around the globe, Atmos. Chem. Phys., 15, 2915-2933, 2015.

B: C_2H_6 and $ClONO_2$ pseudo lines produced by G. C. Toon. Available at https://mark4sun.jpl.nasa.gov/pseudo.html

C: Methane Tikhonov retrieval as defined in: Sussmann, R., et. al: Strategy for high-accuracy-and-precision retrieval of atmospheric methane from the mid-infrared FTIR network, Atmos. Meas. Tech., 4, 1943-1964, 2011

D: CO apriori from: Jones, N. B., et al.(2007), Strato-mesospheric CO measured by a ground-based Fourier Transform Spectrometer over Poker Flat, Alaska: Comparisons with Odin/SMR and a 2-D model, J. Geophys. Res., 112, D20303. WACCMv6 stratospheric CO is too high.

E: The 125HR SNR is less than the 120HR due to two reasons: 125HR spectra is an average of 2 scans, whereas 120HR is an average of 5. The spectral resolution of 120HR spectra (NDACC filter #2) used in HCN analysis is 0.007cm^{-1}, whereas it is 0.0035cm^{-1} for the 125HR.

GAS	Microwindows (cm^{-1})	Spectroscopic database	Interfering species	Apriori	Sa	SNR 120HR (125HR)
O_3	782.56 – 782.86 788.85 – 789.37 894.40 – 896.60 (H_2O only) 993.30 – 993.80 1000.00 – 1005.00	HIT-08	H_2O, CO_2, C_2H_4, $^{668}O_3$, $^{686}O_3$	WACCM refb2.1:[A] average over 1980-2020.	Diagonal: 10%	150 (150)
HNO_3	867.05 – 870.00 872.25 – 874.00	HIT-08	H_2O, OCS, NH_3, H_2O	WACCMv6: average over 1980-2020.	Derived from WACCMv6 climatology	SNR calculated for each spectrum
HF	4038.81 – 4039.07 4109.77 – 4110.07	HIT-08	H_2O, HDO, CH_4	WACCMv6: monthly climatology over 1980-2020.	Diagonal: 50%	270 (320)[B]
HCl	2727.73 – 2727.83 2775.70 – 2775.8 2925.75 – 2926.05	HIT-08	CH_4, HDO, NO_2, O_3, N_2O	WACCMv6: average over 1980-2020.	0-18km: Derived from WACCMv6 climatology 18km+: tapering to 25%	650 (650)[B]
$ClONO_2$	779.05 – 779.90 780.05 – 780.70 780.90 – 781.10	$ClONO_2$ pseudo lines[B]	O_3, H_2O, CO_2, C_2H_6, HNO_3	WACCMv6: Average over 1980-2020.	0- 6km & 30km+: Derived from WACCMv6 climatology 6-30km: 50%	90 (100)
N_2O	2481.30 – 2482.60 2526.40 – 2528.20 2537.85 – 2538.80 2540.10 – 2540.70	HIT-08	CO_2, CH_4 HDO, CO_2	WACCMv6: Average over 1980-2020.	Derived from WACCMv6 climatology	300 (400)
CH_4	2613.70 – 2615.40 2835.50 – 2835.80 2921.00 – 2921.60	HIT-00 + updates	HDO, H_2O, CO_2, NO_2	WACCMv6: average over 1980-2020.	Tikhonov L1[C]	350 (480)
CO	2057.70 – 2058.00 2069.56 – 2069.76 2157.50 – 2159.15	ATM-12	H_2O, O_3, N_2O, CO_2, OCS	Jones et al.[D](2007), JGR	Diagonal: 0- 50km 20% 50km+: tapering to 2%	200 (270)
C_2H_6	2976.66 – 2977.059 2983.20 – 2983.50	C_2H_6 pseudo lines[B]	H_2O, O_3, CH_3Cl, CH_4	Mahieu, pers. comm. Scaled WACCMv6 (x2.4)	Mahieu, pers. comm. Derived from CHASER model	350 (425)
HCN	3268.05 – 3268.40 3287.18 – 3287.35 3299.40 – 3299.60	HIT-08	H_2O, $H2^{18}O$, C_2H_2, CO_2	WACCMv6: average over 1980-2020.	Derived from WACCMv6 climatology	1500 (1000)[E]

Table S1. Summary of the species retrieval parameters.

S2. Summary intercomparison analysis and results per species

Comparison of retrieved species total column per comparison day. The mean total column (TC), number of observations (N) and 1-σ relative standard deviation (SD%) for both measurements are tabulated. The difference in the mean daily column (TC Diff) is relative to the 120HR mean TC ((125-120)/120*100.0). TC Diff SD(%) is the instrument SD% added in quadrature. At the bottom of each table is the mean weighted TC difference (bias) over the entire comparison period (in bold).

O_3		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	318	8.95E+18	4	0.46	8.91E+18	4	0.16	-0.49	0.48
2017	327	8.26E+18	3	0.87	8.16E+18	15	0.16	-1.3	0.88
2017	332	8.35E+18	5	1.17	8.20E+18	20	0.21	-1.79	1.19
2018	23	7.71E+18	5	0.2	7.57E+18	4	0.04	-1.77	0.2
2018	30	7.02E+18	7	2.39	6.85E+18	7	0.13	-2.41	2.39
2018	38	8.12E+18	5	0.54	8.05E+18	15	0.23	-0.78	0.59
2018	49	7.50E+18	2	0.63	7.49E+18	14	0.29	-0.15	0.69
2018	97	7.50E+18	7	0.3	7.47E+18	14	0.27	-0.38	0.4
2018	108	8.95E+18	3	0.15	8.89E+18	12	0.33	-0.67	0.37
mean [nobs weighted] TC difference (%): -1.19									

HNO_3		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	332	1.06E+16	6	2.45	1.06E+16	17	3.72	0.9	0.04
2018	29	9.62E+15	5	4.86	1.03E+16	10	3.35	1.06	7.01
2018	97	1.14E+16	7	2.5	1.20E+16	7	3	1.13	4.78
2018	108	1.54E+16	3	0.92	1.55E+16	12	2.44	0.7	0.49
2018	121	1.39E+16	4	3.21	1.39E+16	12	1.41	0.41	-0.03
mean [nobs weighted] TC difference(%): 2.19									

HF		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	310	1.75E+15	2	1.72	1.74E+15	10	0.21	0.07	-0.87
2017	312	1.81E+15	9	3.19	1.86E+15	12	0.64	0.18	2.49
2017	327	1.13E+15	5	1.16	1.13E+15	15	0.39	0.1	-0.56
2017	352	1.70E+15	10	1.57	1.69E+15	15	1.04	0.27	-0.63
2018	29	1.31E+15	5	0.8	1.31E+15	15	0.38	0.1	0.13
2018	38	1.52E+15	7	1.8	1.52E+15	12	0.29	0.08	0.42
2018	44	1.33E+15	8	4.7	1.31E+15	12	0.35	0.1	-1.49
2018	95	1.36E+15	7	1.58	1.37E+15	12	0.37	0.11	0.59
2018	112	1.59E+15	8	1.57	1.58E+15	12	0.35	0.1	-0.48
mean [nobs weighted] TC difference(%): 0.06									

HCl		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	326	2.91E+15	10	3.24	2.90E+15	13	1.08	0.3	-0.23
2017	327	2.86E+15	14	2.21	2.92E+15	15	1.51	0.39	2.06
2017	352	4.26E+15	6	2.24	4.19E+15	10	1.27	0.4	-1.69
2018	29	3.02E+15	7	2.87	3.16E+15	14	1.1	0.29	4.53
2018	38	3.60E+15	8	1.96	3.66E+15	15	1.58	0.41	1.82
2018	43	2.96E+15	6	1.81	2.99E+15	16	3.67	0.92	0.81
2018	44	3.23E+15	6	3.78	3.23E+15	10	1.54	0.49	0.12
2018	95	3.04E+15	8	0.49	3.09E+15	14	0.62	0.17	1.72
mean [nobs weighted] TC difference(%): 1.19									

$ClONO_2$		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2018	30	6.82E+14	6	15.13	6.84E+14	15	14.33	3.7	0.28
2018	121	7.14E+14	4	14.35	6.17E+14	12	23.4	6.76	-13.53
mean [nobs weighted] TC difference(%): -8.01									

N_2O		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	326	6.57E+18	10	0.46	6.52E+18	13	0.13	0.04	-0.83
2017	327	6.54E+18	15	0.54	6.56E+18	15	0.17	0.05	0.33
2017	352	6.34E+18	6	0.26	6.36E+18	11	0.47	0.14	0.27
2018	29	6.48E+18	7	0.42	6.55E+18	15	0.17	0.04	1.19
2018	38	6.45E+18	8	0.45	6.48E+18	15	0.2	0.05	0.41
2018	43	6.40E+18	8	0.22	6.40E+18	16	0.23	0.06	0
2018	44	6.44E+18	6	0.51	6.44E+18	10	0.27	0.08	0.01
mean [nobs weighted] TC difference(%): 0.16									

CH_4		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	326	3.71E+19	10	0.46	3.71E+19	13	0.07	0.02	0.2
2017	327	3.71E+19	15	0.52	3.74E+19	15	0.12	0.03	0.84
2017	352	3.56E+19	6	0.48	3.58E+19	11	0.34	0.1	0.74
2018	29	3.68E+19	7	0.53	3.70E+19	15	0.12	0.03	0.53
2018	38	3.62E+19	8	0.56	3.63E+19	15	0.18	0.05	0.19
2018	43	3.59E+19	8	0.56	3.61E+19	16	0.12	0.03	0.41
2018	44	3.59E+19	6	0.41	3.61E+19	10	0.54	0.17	0.42
2018	95	3.64E+19	8	0.39	3.65E+19	15	0.18	0.05	0.12
mean [nobs weighted] TC difference(%): 0.46									

CO		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	318	1.30E+18	4	0.84	1.33E+18	3	0.54	0.31	1.65
2017	326	1.35E+18	10	1.41	1.35E+18	15	0.14	0.04	0.19
2018	29	1.16E+18	7	0.91	1.16E+18	15	0.48	0.12	0.25
2018	38	8.72E+17	8	1.35	8.76E+17	15	0.3	0.08	0.44
2018	43	9.66E+17	9	1.76	9.70E+17	20	1.25	0.28	0.41
2018	49	9.28E+17	6	1.14	9.28E+17	15	0.95	0.24	0.02
2018	97	8.12E+17	10	1.44	8.08E+17	15	0.43	0.11	-0.45
mean [nobs weighted] TC difference(%): 0.22									

C_2H_6		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	318	5.60E+15	3	13.22	6.23E+15	3	2.52	1.45	11.28
2017	326	5.37E+15	8	8.34	5.41E+15	13	5.46	1.51	0.66
2017	327	6.29E+15	14	9.29	6.66E+15	15	7.44	1.92	5.96
2017	352	2.24E+15	5	23.8	2.85E+15	11	10.13	3.05	27.46
2018	29	5.49E+15	5	6.13	5.70E+15	15	3.62	0.93	3.81
2018	38	2.62E+15	8	13.58	2.94E+15	15	6.34	1.64	12.24
2018	43	3.03E+15	5	5.1	3.18E+15	15	9.22	2.38	4.92
2018	44	2.73E+15	6	15.41	3.49E+15	10	9.99	3.16	27.85
2018	95	4.73E+15	8	7.43	4.35E+15	13	11.76	3.26	-8.06
mean [nobs weighted] TC difference(%): 8.05									

HCN		120HR			125HR				
YEAR	DOY	TC	N	SD(%)	TC	N	SD(%)	TC Diff(%)	TC Diff SD(%)
2017	318	5.96E+15	6	2.21	6.00E+15	5	1.68	0.75	0.72
2017	327	5.79E+15	7	8.19	5.88E+15	10	1.66	0.52	1.57
2018	29	4.14E+15	6	10.38	3.93E+15	8	3.82	1.35	-5.14
2018	30	4.17E+15	13	5.32	4.15E+15	15	2.42	0.62	-0.61
2018	38	3.43E+15	8	9	3.41E+15	15	2.81	0.72	-0.42
2018	95	2.98E+15	9	9.89	2.88E+15	13	5.06	1.4	-3.32
2018	106	2.34E+15	4	22.45	2.73E+15	12	2.22	0.64	16.96
2018	112	2.43E+15	9	6.84	2.28E+15	15	4.35	1.12	-5.94
2018	121	2.74E+15	2	2.34	2.77E+15	6	3.89	1.59	1.02
mean [nobs weighted] TC difference(%): -0.93									