TNRCC MODELING ASSISTANCE PROJECT II

ASSISTANCE WITH TWIN OTTER DATA MANIPULATION, QUALITY CHECKING, AND PROCESSING FOR THE TexAQS 2000 AIR MEASUREMENT DATA SET

FINAL REPORT
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1. INTRODUCTION

The goal of this work was to improve the quality and confidence level of the Baylor University Twin Otter data set that will be submitted as part of the TexAQS 2000 air quality study and to prepare a self-consistent data set for the flights conducted during TexAQS 2000 for subsequent data analysis. The work focused on the data collected for NO, NO_2, NO_y and NO_y*, but also included critical evaluation of the ozone, CO, and SO_2 data, and physical parameters (temperature, dewpoint, etc). One product of the work was development of a protocol to carry out this evaluation for past, current and future data sets. In that connection the initial work focused on only a few select flights conducted during the TexAQS 2000 study. The primary work product is this report of the evaluation and manipulation of these flights, including the computer programs or algorithms developed, so that the capacity for performing this work can be transferred to the Baylor University research staff. The work included presentation of the results of the initial analysis to the Baylor University staff. This report includes presentation-ready graphics detailing results of the analyses discussed below that can be used by either Baylor University or TNRCC in future presentation of the data.

2. DESCRIPTION OF DATA ANALYSES PERFORMED

2.1 ANALYSES THAT RESULTED IN AN ALGORITHM TO MODIFY THE DATA

2.1.1 True Response Speed

The response speed of the chemical and physical sensors utilized during the study was assessed through analysis of power spectra of the data collected. This information was used to determine the optimal data reporting rates for each measurement. It should not be necessary to repeat this process on a routine basis unless there is some physical change implemented in the sampling system. This analysis was carried out for all of the data collected during 20 morning and afternoon flights, which were compiled into one database (approximately 87,000 1-second observations during the morning flights and 106,000 1-second observations collected during the afternoon flights).

The analysis was performed by plotting the signal squared (e.g. $[NO]^2$) versus the frequency response arrived at via Fourier transform of the data. Because of sampling statistics (Nyquist frequency) the fastest possible response speed is one-half of the data collection rate. Since the data were recorded at 1 Hz, this value is 0.5 Hz. An ideal signal would show a –3/2 slope up to the frequency where the signal was dominated by noise. In practice, the plots necessary for this analysis were produced using a procedure written in Igor Pro that depends largely on an existing power spectral density procedure that is included in the Igor Pro software package. The procedure and a description of its implementation are included in Appendix A. The optimal data reporting frequency was determined by examining the frequency response of all of the sensors to identify the slowest measurement and its true response speed.

In addition to examination of the frequency response of a signal, this analysis was used to identify possible sampling artifacts in the signal. This was accomplished by comparing the frequency response of the various instruments during morning and afternoon flights with the assumption that the air composition was significantly different between the two periods. The results of this analysis are shown graphically in **Figures 2-1 through 2-6**.

The slowest responding sensor was determined to be the SO_2 instrument, with a response speed of about 0.2 Hz (5 seconds). Based on this result, the optimal data reporting frequency is 5-second data. Also resulting from this analysis is an indication of slower response speed for the NO_y and NO_y* measurements under conditions that may have higher HNO_3 abundance.

2.1.2 Optimal Data Reporting Frequency

The result of the work discussed in Section 2.1.1 indicated that the SO_2 sensor was the slowest responding instrument at about 0.2 Hz. To produce a database that considers all parameters on an equal basis, a procedure was written to produce a 5-second averaged database. This procedure and a brief discussion of its implementation are included in Appendix A.

2.1.3 Time Shift for All Parameters

The time shifts performed on the data received for this analysis were determined initially to be adequate to represent the time lags experienced between the different sensors because of differences in sample inlet length, flow rates, and internal signal processing. Subsequent review of the data showed that on a flight-by-flight basis, the time shifts required to align peaks and valleys varied somewhat. To more readily adjust for these variations, a procedure was written in Igor Pro that allows for fine-tuning of the time shift for an individual flight. That procedure is discussed in more detail in Appendix A.

2.1.4 Water Vapor Corrections

The chemiluminescent sensors have a well-documented sensitivity dependence on water vapor. The effect is such that the dry sensitivity (measured with zero air displacement calibrations) is higher than that realized in moist ambient air. The magnitude of the correction is 0.4%/ppth H_2O. A data reduction procedure was developed in Igor Pro to apply this correction to the data in the form:

Fasto3_ppbv_cor = FastO3_ppbv+(FastO3_ppbv*(.004*H_2O))

A similar correction was performed for all of the sensors based on NO + O_3 chemiluminescence (NO, NO_2, NO_y, NO_y*, O_3). The water vapor concentration required for this correction was calculated based on measured ambient temperature and dewpoint. A procedure to calculate water vapor is included with other procedures discussed in Appendix A.

2.2 ANALYSES THAT RESULTED IN QUANTITATIVE DATA DESCRIPTION

2.2.1 Hysteresis

The occasion of hysteresis in the NO_y measurement was addressed in two different ways. First, as discussed in Section 2.1.1, the power spectra for NO_y and NO_y* showed a somewhat slower response speed during the morning sampling periods than in the afternoon. This could result from either sampling of photochemically aged air masses in the morning that had a higher abundance of HNO_3, leading to slower response speed, or a reduced response speed because of presumably cooler sample inlets in the morning. In either case, the net result is a small sampling hysteresis when transitioning from a relatively polluted to a relatively clean air parcel.

This issue was also explored by plotting an up and down vertical profile performed at the same location. Sampling hysteresis can be examined by comparison of the polluted-to-clean and clean-to-polluted transitions. Vertical profiles like this were performed regularly by the Twin Otter over Galveston Bay. An example is shown in **Figure 2-7**. Similar vertical profile pairs were examined for other flights. The overall conclusion is that there does seem to be some hysteresis when transitioning from polluted to clean atmospheres. For future measurements, this effect can be minimized by employing heaters on the Teflon inlet tubes.

2.2.2 Precision and Accuracy

An uncertainty budget for each of the trace gas measurements was estimated assuming a normal distribution of errors. The categories of error considered are shown in **Table 2-1**. The effects that the uncertainties listed in Table 2-1 have on the data quality is best shown graphically. **Figures 2-8 and 2-9** show selected time series for ozone and NO_y respectively, along with the calculated 1σ uncertainty limits.

With the exception of the CO measurement, the uncertainties listed only limit the utility of the data at lower concentrations. Since the primary purpose of this set of measurements was to explore emissions from different source types, the fact that the quality of the data degrades as the levels approach the lower end may not affect the usefulness of the data.

The difficulty with the CO measurement is that there were large uncertainties in the system sensitivity as well as the baseline. This leads to both a large percentage uncertainty and a large fixed uncertainty. Ground-based calibrations and inter-comparisons conducted in zero air indicated that the instrument could measure CO reasonably. The difficulty came with the lack of zero and sensitivity determinations in ambient air. Comparison of the reported CO values with canister samples collected on the Twin Otter shows literally no correlation. In spite of this fact, the CO instrument did respond to CO when it was expected to (e.g., in an urban plume) and showed relatively more signal in the mixed layer than in the free troposphere. Thus the variation of the CO signal may still be of utility in defining different air mass types and composition.

Table 2-1. Uncertainty budget for the chemical parameters measured aboard the Twin Otter during TexAQS 2000.

Parameter	Calibration standard [1]	Conversion efficiency [2]	Repeatability [3]	Baseline [4]	Combined uncertainty [5]
UV Ozone (slow)	5%	N/A	6%	1 ppb	8% + 1 ppb
Chemiluminescent Ozone (fast)	5%	N/A	15%	2 ppb	16% + 2 ppb
NO_y	6%	20%	3%	4 ppb	21% + 4 ppb
NO_y*	6%	3%	3%	6 ppb	7 % + 6 ppb
NO2	6%	8%	4%	3 ppb	11% + 3 ppb
NO	4%	N/A	3%	1 ppb	5% + 1 ppb
SO_2	4%	N/A	9%	0.3 ppb	10% + 0.3 ppb
CO	4%	N/A	127%	48 ppb	130% + 48 ppb

1 Uncertainty about the calibration standard includes uncertainty about the gas mixture and dilution. For ozone (also the NO_2 calibrations produced using ozone), the uncertainty reflects the variation in the ozone source.
2 For NO_2 and NO_y* the uncertainty in conversion efficiency is estimated from repeated calibrations. For NO_y, an additional uncertainty was estimated since HNO_3 conversion efficiency was not determined.
3 The repeatability uncertainty was estimated from the standard deviation of the slopes from approximately 65 calibrations conducted during the study.
4 The uncertainty in the baseline, or zero level of the measurements, was estimated from the standard deviation of the zero level determinations (synthetic air) conducted during the study. Although the measurements were corrected from the zero level, this number reflects the expected variability of that level during ambient measurements.
5 The combined uncertainty was estimated through propagation of the above uncertainties as $((\delta_1)^2 + (\delta_2)^2 + (\delta_n)^2)^{1/2}$.

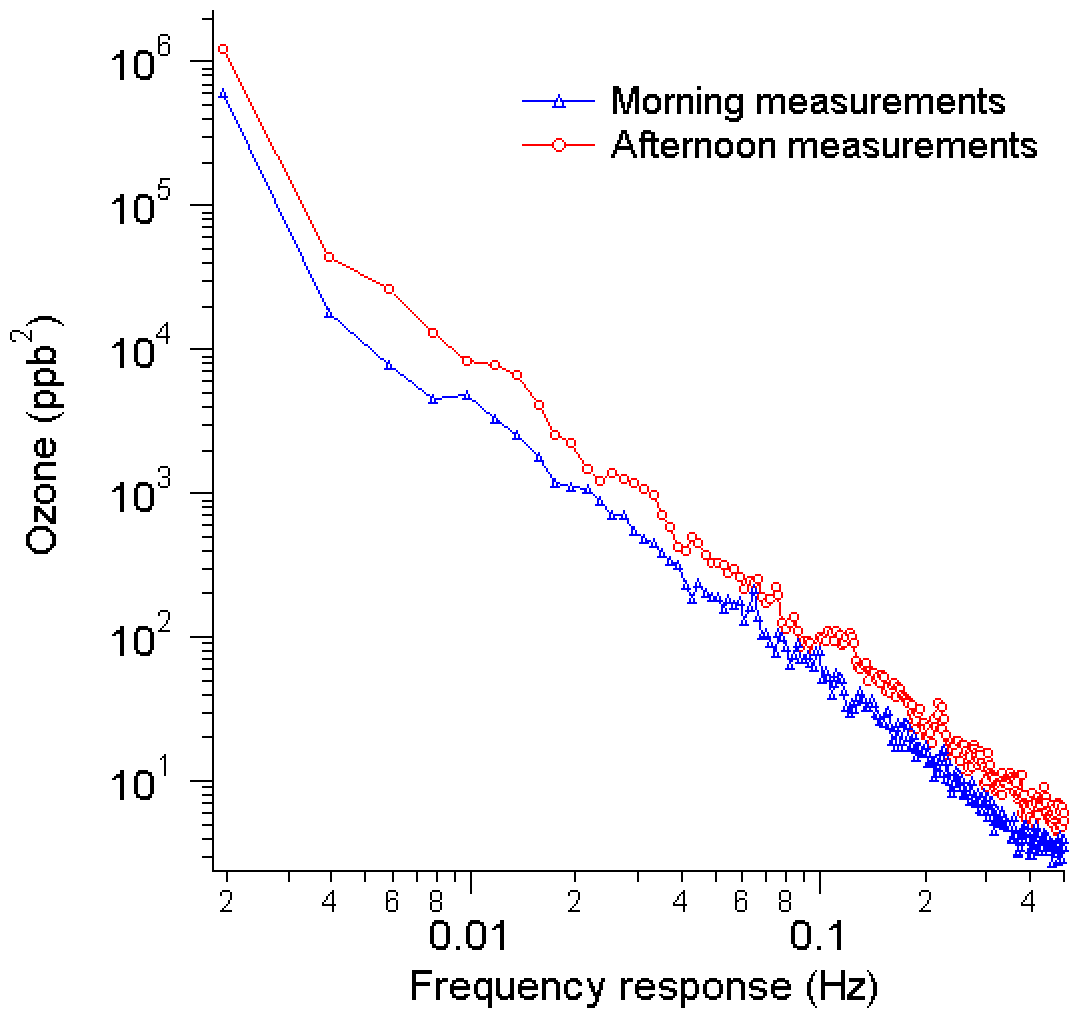

Figure 2-1. Power spectrum of the ozone data collected using the chemiluminescence instrument. This instrument demonstrated very good frequency response up to the maximum 0.5 Hz for the afternoon measurements. The morning measurements indicated slightly slower response speed (~0.4 Hz), indicated by the inflection point in the curve at that frequency.

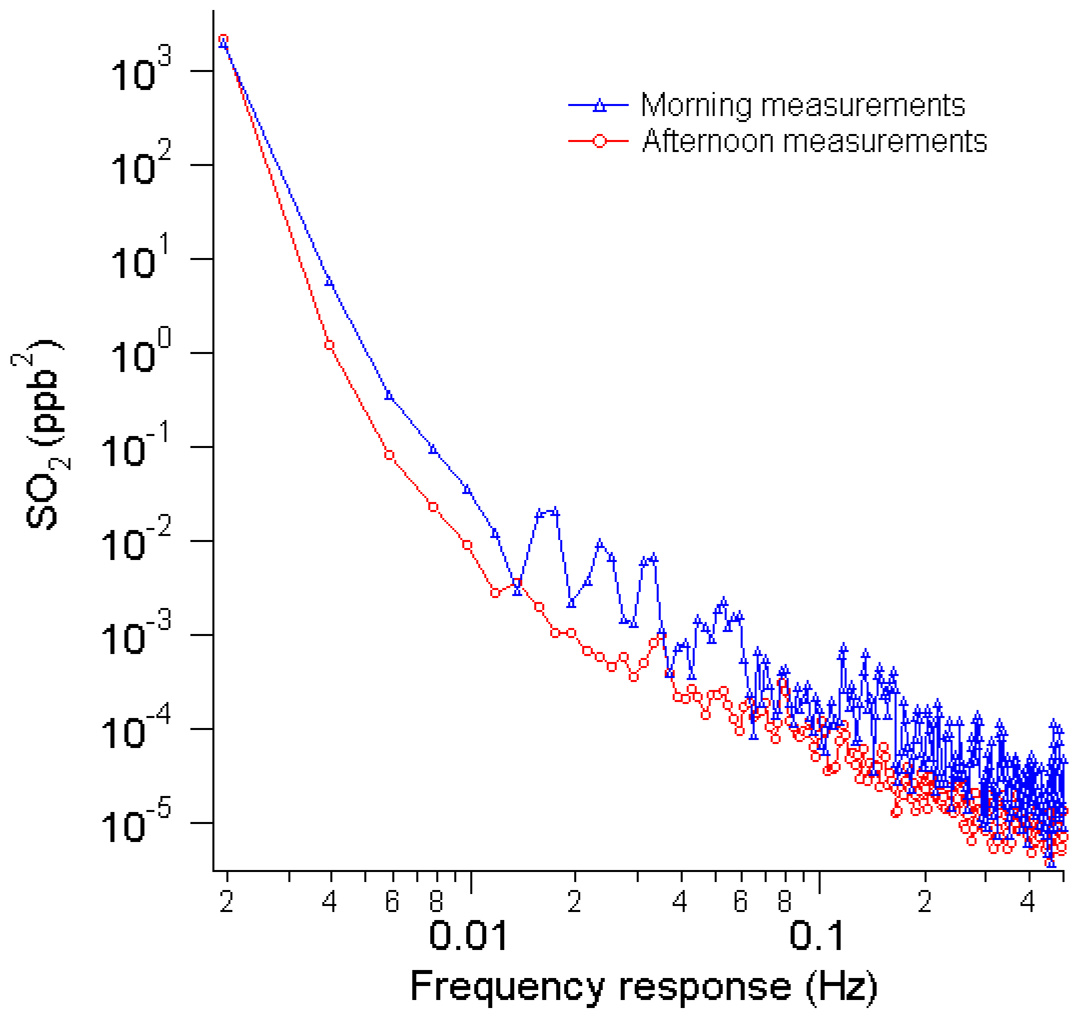

Figure 2-2. Power spectrum of the SO_2 data collected. This instrument demonstrated reasonable frequency response up to about 0.2 Hz for the afternoon measurements. The morning measurements indicated slightly slower response speed, indicated by the inflection point in the curve at 0.1 Hz. Deviation from a straight line at frequencies less than 0.01 Hz is probably due to the infrequent sampling of plumes at high concentrations.

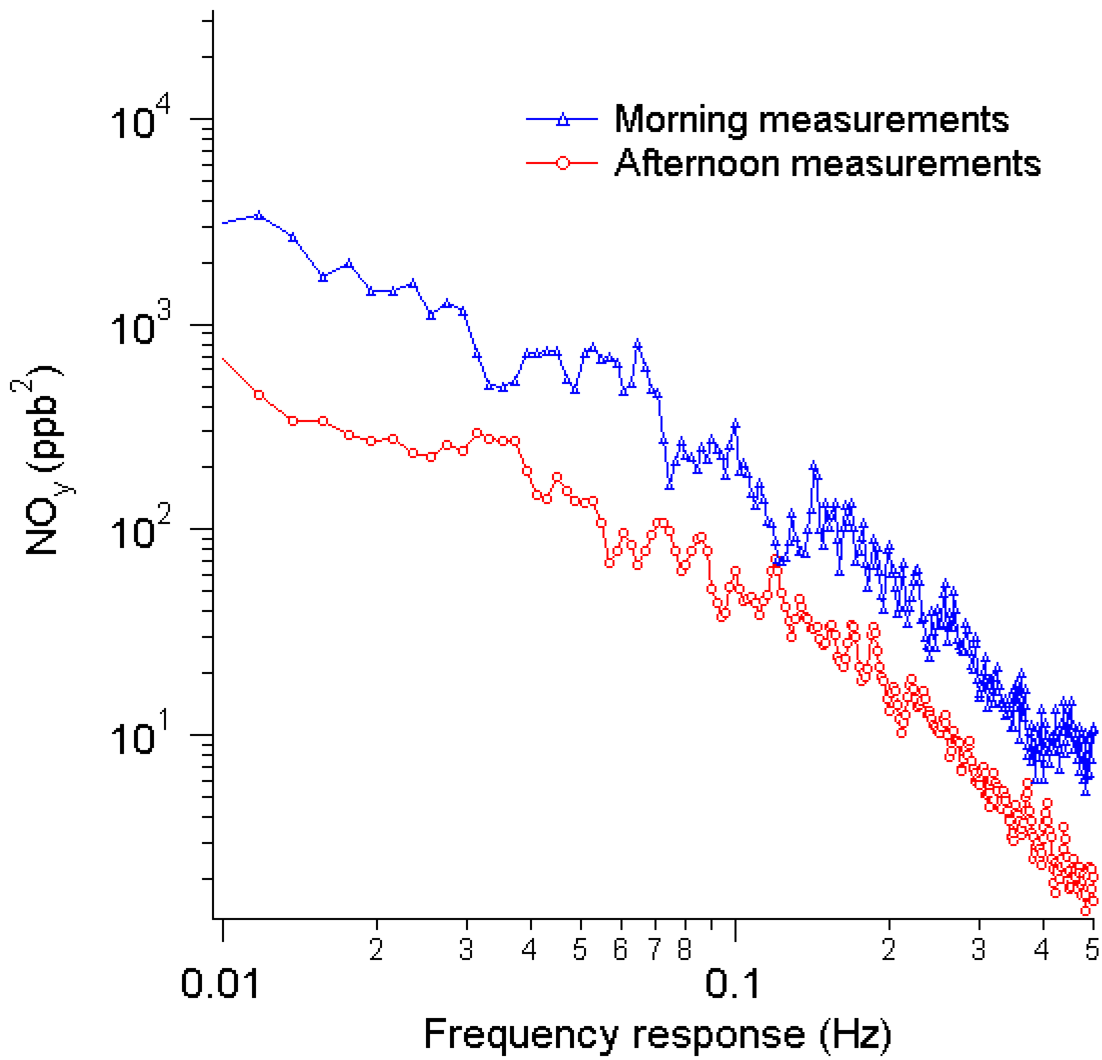

Figure 2-3. Power spectrum of the NO_y data collected using the chemiluminescence instrument. This instrument demonstrated reasonable frequency response up to the maximum 0.4 Hz for both the morning and afternoon measurements. The morning measurements show a more pronounced roll-off into noise at 0.4 Hz. This may result from sampling of photochemically aged air masses aloft that contained more nitric acid than typically observed in the afternoon observations. It is not clear why the NO_y signal was not more linear throughout the range of frequencies observed.

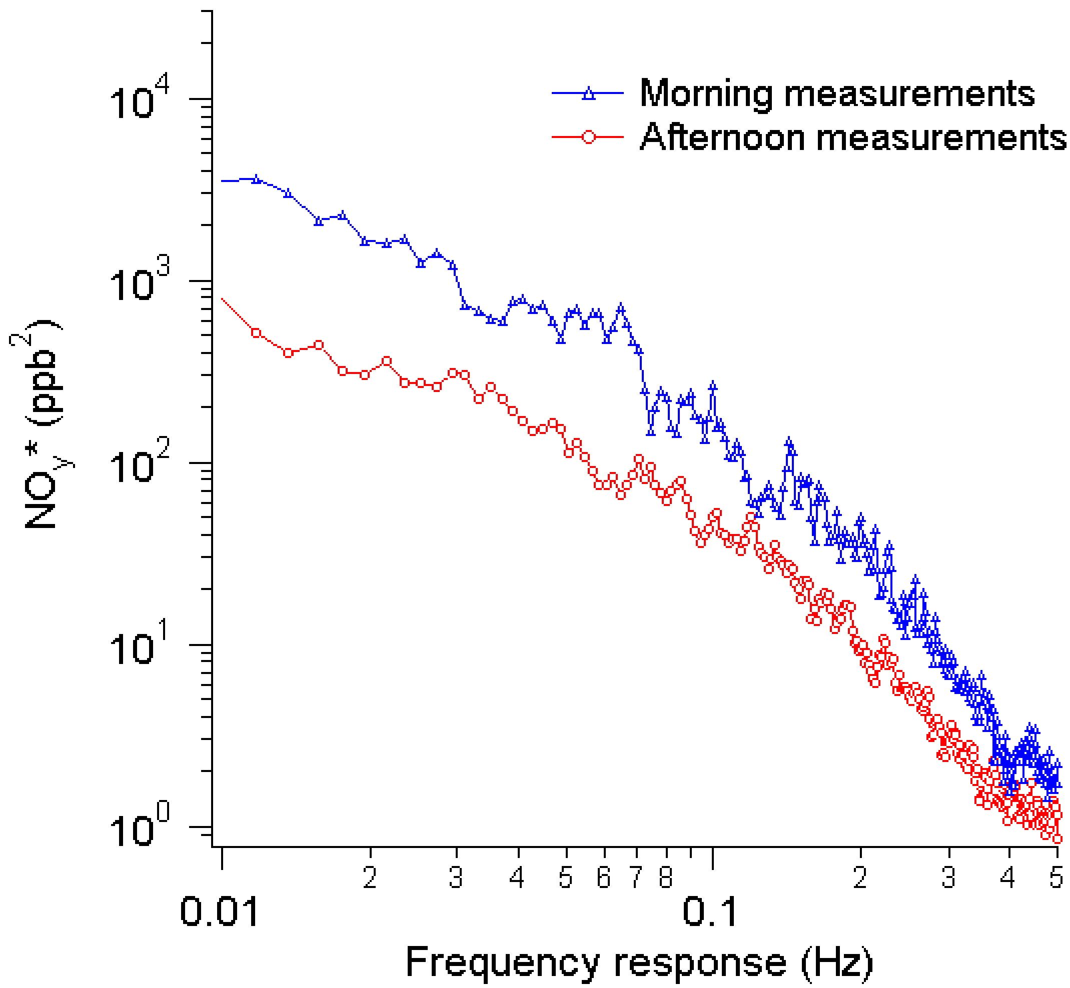

Figure 2-4. Power spectrum of the NO_y* data collected. This instrument demonstrated reasonable frequency response up to 0.4 Hz for both the morning and afternoon measurements. The same more pronounced inflection point in the morning measurements discussed in connection with the NO_y measurement is evidenced here.

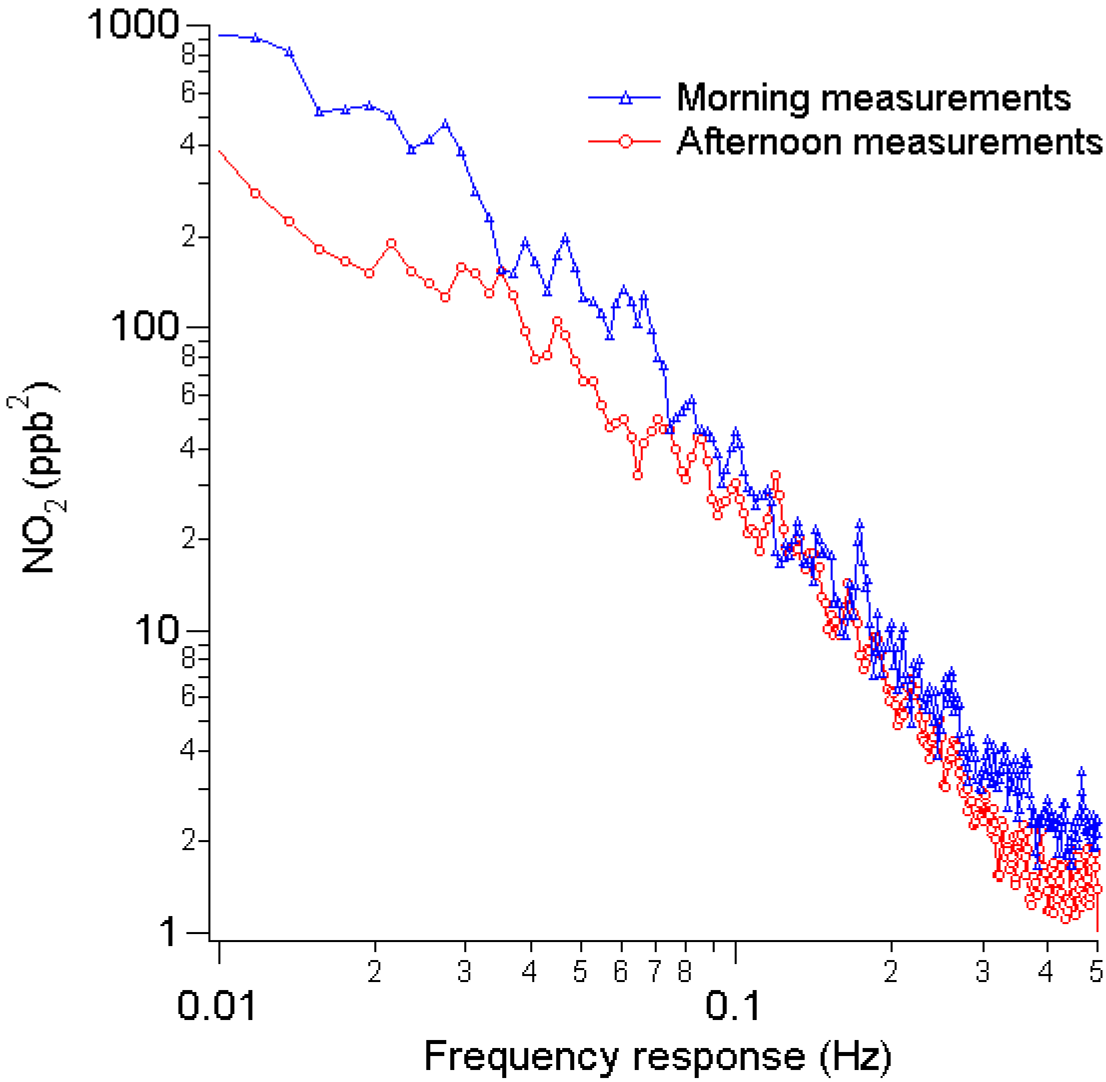

Figure 2-5. Power spectrum of the NO_2 data collected. This instrument demonstrated very good frequency response up to 0.4 Hz for both the morning and afternoon measurements. This result is significant because the NO_2 photolysis cell had a volume that resulted in a 15-second residence time. The indicated response speed of ~2.5 seconds (1/0.4 Hz) suggests that flow through the cell was essentially plug-flow, with minimal longitudinal mixing that would have resulted in a slower response speed.

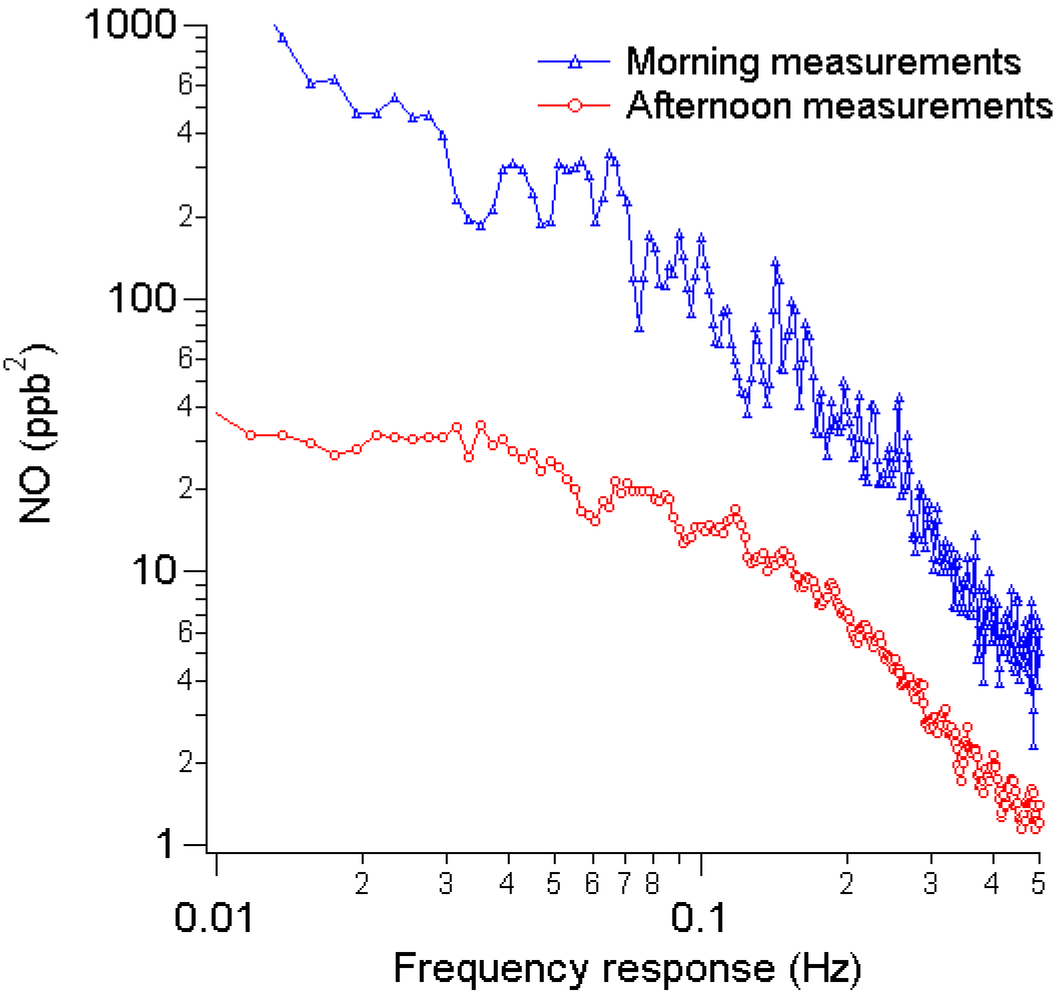

Figure 2-6. Power spectrum of the NO data collected. This instrument demonstrated reasonable frequency response up to about 0.4 Hz for both the morning and afternoon measurements. It is not clear why the morning measurements show better linearity throughout the frequencies observed than do the afternoon measurements.

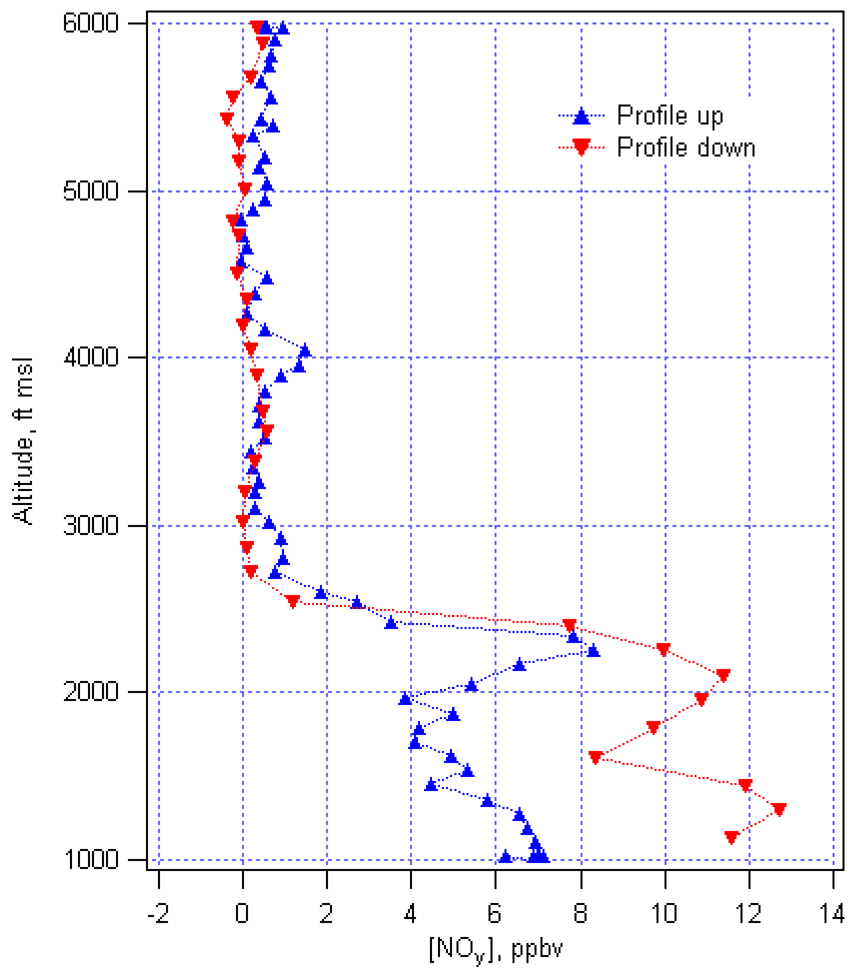

Figure 2-7. Vertical profile collected on the afternoon of August 29, 2000 (flight 143b) over Galveston Bay. The up and down legs of the profile were collected at approximately the same location. Comparison of the transition first out of (Profile up) and then into (Profile down) the mixed layer at approximately 2500 ft indicates that there may be some hysteresis, or memory effect, in the transition from polluted to clean atmospheres, evidenced by the higher NO_y values observed above the boundary layer on the profile up relative to the profile down. This assessment must be tempered by the fact that temporal variation in the NO_y signal was substantial, evidenced by the difference in NO_y abundance observed within the boundary layer. The time difference between the start of the profile up and end of the profile down was 17 minutes.

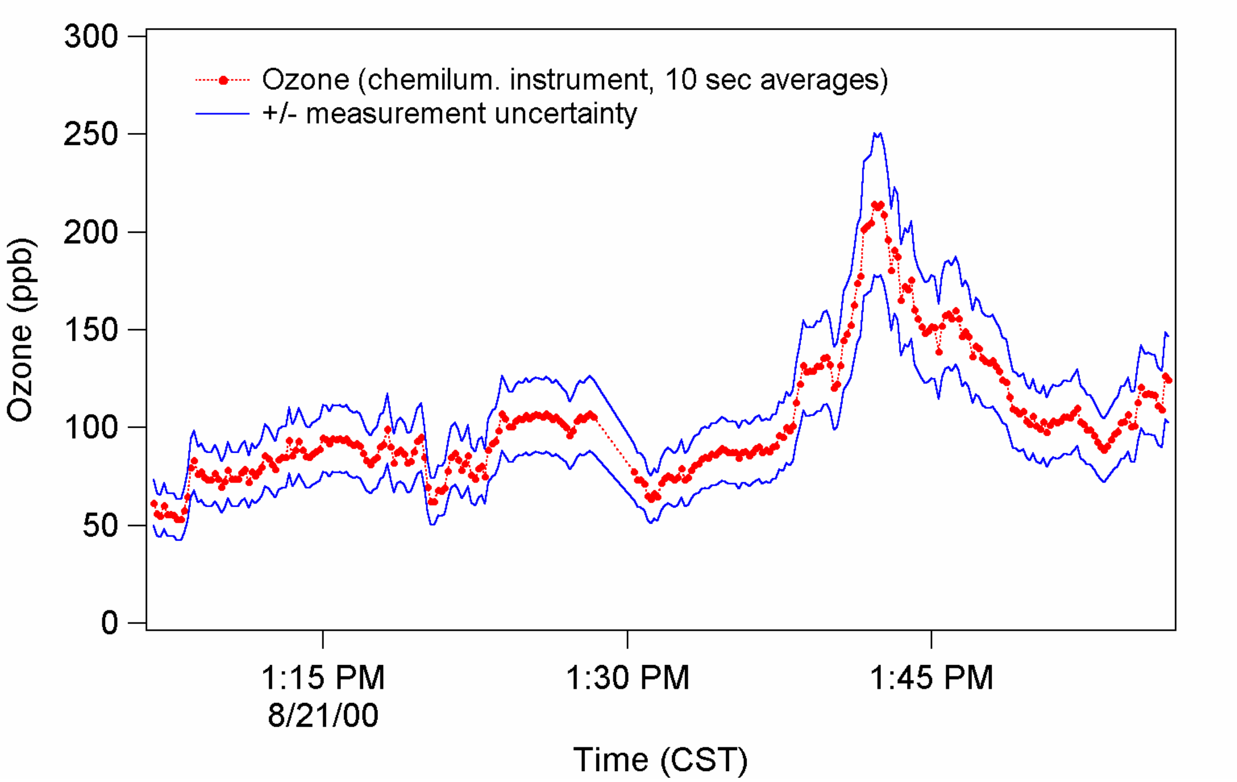

Figure 2-8. Example time series of 10-second average ozone data with 1σ uncertainty limits.

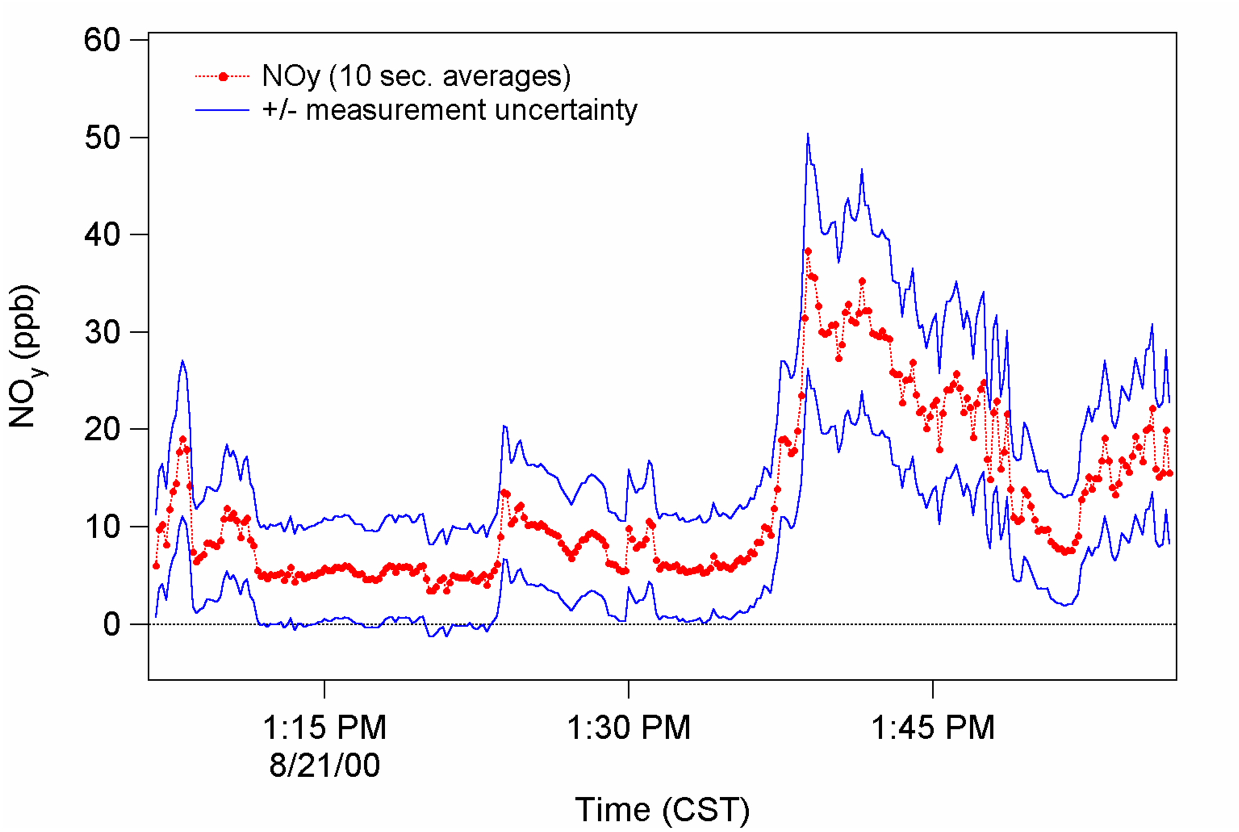

Figure 2-9. Example time series of 10-second average NO_y data with 1σ uncertainty limits.

3. SUMMARY

The trace gas instrumentation operated on the Baylor University Twin Otter had adequate sensitivity and response speed to characterize most of the air parcels observed during the TexAQS 2000 study. With the exception of the CO measurement, which is still under evaluation, the uncertainty associated with each measurement is within reason.

Current work is aimed at decreasing the measurement uncertainty through implementation of automatic, ambient air, zero level determinations. Utilization of the automatic matrix zeros is expected to substantially reduced the fixed offset of the uncertainty estimate, but will have little effect on the uncertainty that stems from calibrations, conversion efficiency, and repeatability. This change in the operation of the instrument will also require additional data processing routines.

Additional recommendations to improve the quality of the data include HNO_3 calibrations of the NO_y sensor, which will serve to better establish the conversion efficiency uncertainty, and heating of the NO_y and NO_y* Teflon inlets to improve the sample transmission speed.

APPENDIX A

IGOR PRO PROCEDURES DEVELOPED FOR DATA PROCESSING

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IGOR PRO PROCEDURES

INTRODUCTION

A series of procedures were written for the Igor Pro computer program to enable automated and/or reproducible processing of the Baylor University Twin Otter data. The procedures are mostly menu driven. A brief description of the various procedures and the working computer code (useful for process and computation evaluation) is included here.

DATA PROCESSING PROCEDURES

Several procedures were written to allow reading and rapid evaluation of the data from the Twin Otter aircraft instrument package. When these procedures are included in the //IgorPro Procedures folder they appear on a pull-down menu on the top menu bar of the program window. This is shown in **Figure A-1** (screen capture from Igor Pro). The following procedures are available from this menu:

ReadTwinOtterFile. This procedure imports the .eng format of the Twin Otter data, produces a time field compatible with Igor Pro, and replaces the –99 no data indicator with not-a-number (NAN) that is more conducive to data plotting.

MakeTOTSplots. This procedure makes a series of time series and flight path plots from the raw data, allowing rapid review of the flight results.

PowerSpectrum. This procedure makes a power spectral density plot from the parameter selected by the user in a menu initated by the procedure.

CalcWater_TO. This procedure calculates the water vapor mixing ratio based on the ambient temperature and dewpoint parameters in the Twin Otter data set.

Water_correction. This procedure applies the water correction to the $NO+O_3$ chemiluminescence instruments using the mixing ratio calculated in CalcWater_TO.

Generate_AvgData. This procedure creates a start-time/stop-time wave and averages the chemical parameters. It also generates a wave of the averaged data distributed at the start-time of the 1-second data.

MakepathsTO. This is a utility procedure that creates the final data file name and path for saving.

WriteNewFieldsTO. This procedure writes a tab-delimited file of the reprocessed data suitable for appending back into the original .eng file. This procedure also converts the QC codes to their NARSTO equivalents.

Additional procedures are available under the EditData pull-down menu shown in **Figure A-2**. These include EnterCalFactors and EnterTimeShifts, both of which present windows to enter the appropriate data for a given flight (also shown in Figure A-2). Finally, a procedure titled ReduceNO2 was written to calculate the true NO_2 concentration based on the input NO_x, NO, and ozone values.

The computer code written for these procedures follows.

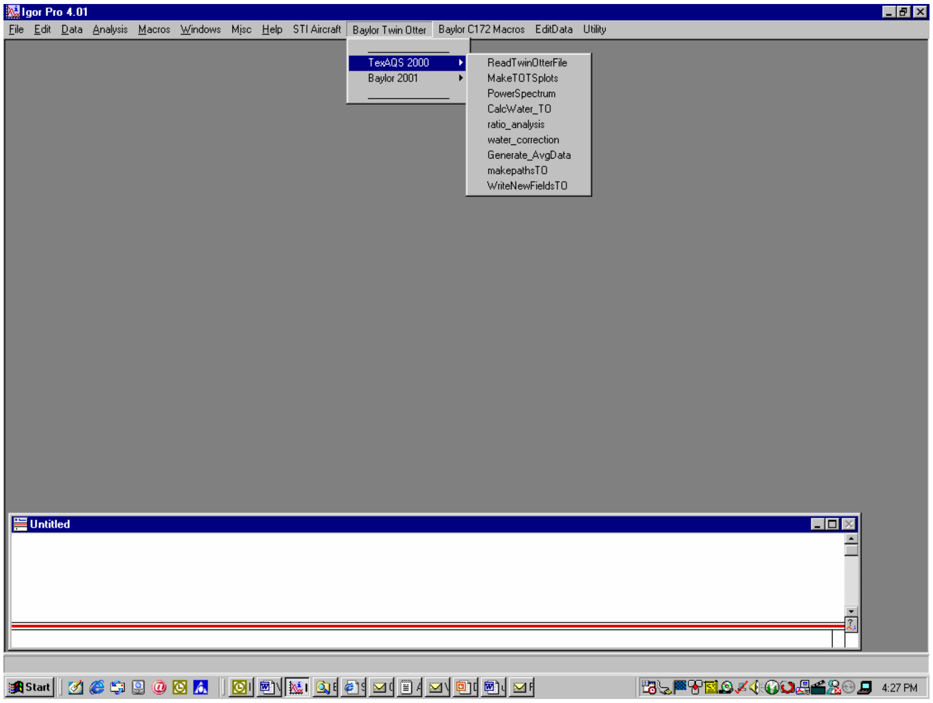

Figure A-1. Screen capture from Igor Pro showing the TexAQS 2000 data processing procedure menu.

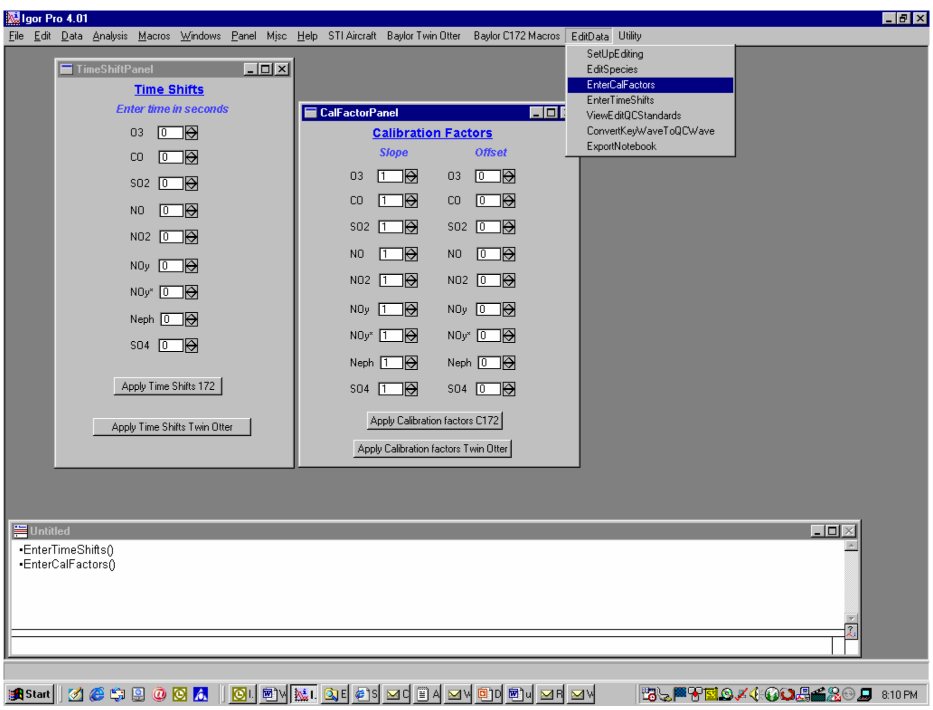

Figure A-2. Screen capture from Igor Pro showing the additional data processing procedures used for the TexAQS 2000 data.

IGOR PRO PROCEDURE CODE

```
#pragma rtGlobals=1		// Use modern global access method.

#include <Strings as Lists>
#include<String Substitution>
#include<Remove Points>

//*****************************************************************************
macro ReadTwinOtterFile()

variable fNum,numHeadLines=0
string inStr, inStrType, columnInfoStr
string/g current_file
open /r /d /T="????" fNum				// select a file via the dialog but don't actually open it yet
open /r fNum as S_fileName		// open a file using the string S_filename that was set during the previous open command

silent(1)

Killwaves/A/Z

close fNum		// close the file

columnInfoStr+="C=1,F=0,N=DATEW_MMDD;"
columnInfoStr+="C=1,F=0,N=TIMEW_HHMMSS;"
columnInfoStr+="C=1,F=0,N=REC_number;"
columnInfoStr+="C=1,F=0,N=Event_flag;"
columnInfoStr+="C=1,F=-2,N=Loran_flag;"
columnInfoStr+="C=1,F=0,N=LAT_deg;"
columnInfoStr+="C=1,F=-2,N=LAT_QC;"
columnInfoStr+="C=1,F=0,N=LON_deg;"
columnInfoStr+="C=1,F=-2,N=LON_QC;"
columnInfoStr+="C=1,F=0,N=Altitude_ft;"
columnInfoStr+="C=1,F=-2,N=Altitude_ft_QC;"
columnInfoStr+="C=1,F=0,N=Altitude_m;"
columnInfoStr+="C=1,F=-2,N=Altitude_m_QC;"
columnInfoStr+="C=1,F=0,N=FastO3_ppbv;"
columnInfoStr+="C=1,F=-2,N=FastO3_QC;"
columnInfoStr+="C=1,F=0,N=NOy_ppbv;"
columnInfoStr+="C=1,F=-2,N=NOy_QC;"
columnInfoStr+="C=1,F=0,N=NOyStar_ppbv;"
columnInfoStr+="C=1,F=-2,N=NOyStar_QC;"
columnInfoStr+="C=1,F=0,N=NO2_ppbv;"
columnInfoStr+="C=1,F=-2,N=NO2_QC;"
```

```
columnInfoStr+="C=1,F=0,N=NO_ppbv;"
columnInfoStr+="C=1,F=-2,N=NO_QC;"
columnInfoStr+="C=1,F=0,N=SO2_ppbv;"
columnInfoStr+="C=1,F=-2,N=SO2_QC;"
columnInfoStr+="C=1,F=0,N=Pres_mb;"
columnInfoStr+="C=1,F=-2,N=Pres_QC;"
columnInfoStr+="C=1,F=0,N=DewPoint_degC;"
columnInfoStr+="C=1,F=-2,N=DewPoint__QC;"
columnInfoStr+="C=1,F=0,N=SlowO3_ppbv;"
columnInfoStr+="C=1,F=-2,N=SlowO3_QC;"
columnInfoStr+="C=1,F=0,N='Bsp_Mm-1';"
columnInfoStr+="C=1,F=-2,N=bsp_QC;"
columnInfoStr+="C=1,F=0,N='Gsp_Mm-1';"
columnInfoStr+="C=1,F=-2,N=Gsp_QC;"
columnInfoStr+="C=1,F=0,N='Rsp_Mm-1';"
columnInfoStr+="C=1,F=-2,N=Rsp_QC;"
columnInfoStr+="C=1,F=0,N='Bbsp_Mm-1';"
columnInfoStr+="C=1,F=-2,N=Bbsp_QC;"
columnInfoStr+="C=1,F=0,N='Gbsp_Mm-1';"
columnInfoStr+="C=1,F=-2,N=Gbsp_QC;"
columnInfoStr+="C=1,F=0,N='Rbsp_Mm-1';"
columnInfoStr+="C=1,F=-2,N=Rbsp_QC;"
columnInfoStr+="C=1,F=0,N=NephP_mb;"
columnInfoStr+="C=1,F=-2,N=NephP_QC;"
columnInfoStr+="C=1,F=0,N=NephSAM_K;"
columnInfoStr+="C=1,F=-2,N=NephSAM_QC;"
columnInfoStr+="C=1,F=0,N=NephInlt_K;"
columnInfoStr+="C=1,F=-2,N=NephInlt_QC;"
columnInfoStr+="C=1,F=0,N='NephRH_%';"
columnInfoStr+="C=1,F=-2,N=NephRH_QC;"
columnInfoStr+="C=1,F=0,N=IAS_kts;"
columnInfoStr+="C=1,F=-2,N=IAS_QC;"
columnInfoStr+="C=1,F=0,N=TAS_kts;"
columnInfoStr+="C=1,F=-2,N=TAS_QC;"
columnInfoStr+="C=1,F=0,N=PALT_ft;"
columnInfoStr+="C=1,F=-2,N=PALT_QC;"
columnInfoStr+="C=1,F=0,N=DALT_ft;"
columnInfoStr+="C=1,F=-2,N=DALT_QC;"
columnInfoStr+="C=1,F=0,N=OAT_degC;"
columnInfoStr+="C=1,F=-2,N=OAT_QC;"
columnInfoStr+="C=1,F=0,N=TAT_degC;"
columnInfoStr+="C=1,F=-2,N=TAT_QC;"
columnInfoStr+="C=1,F=0,N=WDIR_deg;"
columnInfoStr+="C=1,F=-2,N=WDIR_QC;"
columnInfoStr+="C=1,F=0,N=WSPD_kts;"
columnInfoStr+="C=1,F=-2,N=WSPD_QC;"
```

```
columnInfoStr+="C=1,F=0,N=HDNG_deg;"
columnInfoStr+="C=1,F=-2,N=HDNG_QC;"
columnInfoStr+="C=1,F=0,N=ValveTime_sec;"
columnInfoStr+="C=1,F=-2,N=ValveTime_QC;"
columnInfoStr+="C=1,F=0,N=CellInd_ascii;"
columnInfoStr+="C=1,F=-2,N=CellInd_ascii_QC;"
columnInfoStr+="C=1,F=0,N=RHvolts_vdc;"
columnInfoStr+="C=1,F=-2,N=RHvolts_QC;"
columnInfoStr+="C=1,F=0,N=TMPvolts_vdc;"
columnInfoStr+="C=1,F=-2,N=TMPvolts_QC;"
columnInfoStr+="C=1,F=0,N=FMvolts_vdc;"
columnInfoStr+="C=1,F=-2,N=FMvolts_QC;"
columnInfoStr+="C=1,F=0,N=VoltDP_vdc;"
columnInfoStr+="C=1,F=-2,N=VoltDP_QC;"
columnInfoStr+="C=1,F=0,N=CellSig_vdc;"
columnInfoStr+="C=1,F=-2,N=CellSig_QC;"
columnInfoStr+="C=1,F=0,N=CellBase_vdc;"
columnInfoStr+="C=1,F=-2,N=CellBase_QC;"
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columnInfoStr+="C=1,F=-2,N=Temp_QC;"
columnInfoStr+="C=1,F=0,N=CT_degC;"
columnInfoStr+="C=1,F=-2,N=CT_QC;"
columnInfoStr+="C=1,F=0,N='CellSigCellBASE_ng/l';"
columnInfoStr+="C=1,F=-2,N=CellSigCellBASE_QC;"
columnInfoStr+="C=1,F=0,N=CO_ppbv;"
columnInfoStr+="C=1,F=-2,N=CO_QC;"
//columnInfoStr+="C=1,F=0,N=NO2_uncal_ppbv;"
//columnInfoStr+="C=1,F=-2,N=NO2_uncal_QC;"
//columnInfoStr+="C=1,F=0,N=NOy_smth_ppbv;"
//columnInfoStr+="C=1,F=-2,N=NOy_smth_QC;"
//columnInfoStr+="C=1,F=0,N=NOyStar_smth_ppbv;"
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//columnInfoStr+="C=1,F=0,N=NO_smth_ppbv;"
//columnInfoStr+="C=1,F=-2,N=NO_smth_QC;"
//columnInfoStr+="C=1,F=0,N=O3_smth_ppbv;"
//columnInfoStr+="C=1,F=-2,N=O3_smth_QC;"
//columnInfoStr+="C=1,F=0,N=TotalNitrate_ppbv;"
//columnInfoStr+="C=1,F=-2,N=TotalNitrate_QC;"
columnInfoStr+="C=1,F=-2,N=NAME;"
columnInfoStr+="C=1,F=-2,N=PATH;"
columnInfoStr+="C=1,F=-2,N=LOC;"
columnInfoStr+="C=1,F=-2,N=PASS;"

LoadWave/Q/A/J/D/L={2,3,0,0,0}/B=columnInfoStr S_fileName

Change2Nan()
```

```
Maketimewave()
current_file=S_fileName
print current_file

endmacro

//**************************************************************************
//This macro changes the -99 values to not-a-number (nan) to facilitate plotting and averaging

Macro Change2Nan()

Change992nans(DATEW_MMDD,-99)
Change992nans(TIMEW_HHMMSS,-99)
Change992nans(REC_number,-99)
Change992nans(Event_flag,-99)
Change992nans(LAT_deg,-99)
Change992nans(LON_deg,-99)
Change992nans(Altitude_ft,-99)
Change992nans(Altitude_m,-99)
Change992nans(FastO3_ppbv,-99)
Change992nans(NOy_ppbv,-99)
Change992nans(NOyStar_ppbv,-99)
Change992nans(NO2_ppbv,-99)
Change992nans(NO_ppbv,-99)
Change992nans(SO2_ppbv,-99)
Change992nans(Pres_mb,-99)
Change992nans(DewPoint_degC,-99)
Change992nans(SlowO3_ppbv,-99)
Change992nans('Bsp_Mm-1',-99)
Change992nans('Gsp_Mm-1',-99)
Change992nans('Rsp_Mm-1',-99)
Change992nans('Bbsp_Mm-1',-99)
Change992nans('Gbsp_Mm-1',-99)
Change992nans('Rbsp_Mm-1',-99)
Change992nans(NephP_mb,-99)
Change992nans(NephSAM_K,-99)
Change992nans(NephInlt_K,-99)
Change992nans('NephRH_%',-99)
Change992nans(IAS_kts,-99)
Change992nans(TAS_kts,-99)
Change992nans(PALT_ft,-99)
Change992nans(DALT_ft,-99)
Change992nans(OAT_degC,-99)
Change992nans(TAT_degC,-99)
Change992nans(WDIR_deg,-99)
Change992nans(WSPD_kts,-99)
```

```
Change992nans(HDNG_deg,-99)
Change992nans(ValveTime_sec,-99)
Change992nans(CellInd_ascii,-99)
Change992nans(RHvolts_vdc,-99)
Change992nans(TMPvolts_vdc,-99)
Change992nans(FMvolts_vdc,-99)
Change992nans(VoltDP_vdc,-99)
Change992nans(CellSig_vdc,-99)
Change992nans(CellBase_vdc,-99)
Change992nans(Temp_degC,-99)
Change992nans(CT_degC,-99)
//Change992nans('CellSigCellBASE_ng/l',-99)
//Change992nans(NO2_uncal_ppbv,-99)
Change992nans(CO_ppbv,-99)
//Change992nans(NO2_uncal_ppbv,-99)
//Change992nans(NOy_smth_ppbv,-99)
//Change992nans(NOyStar_smth_ppbv,-99)
//Change992nans(NO_smth_ppbv,-99)
//Change992nans(O3_smth_ppbv,-99)
//Change992nans(TotalNitrate_ppbv,-99)
//Change992nans(PASS,-99)

endmacro

//***************************************************************************

Macro MakeTimewave()

Duplicate/O timeW_HHMMSS, hour,minute,second
hour=((timeW_HHMMSS-mod(timeW_HHMMSS,10000))/1e4)
minute=(mod(timeW_HHMMSS,10000)-mod(timeW_HHMMSS,100))/100
second=mod(timeW_HHMMSS,100)

Duplicate/O DATEW_MMDD year,month,day

year=(DATEW_MMDD-mod(DATEW_MMDD,10000))/10000+2000
month=(mod(DATEW_MMDD,10000)-mod((DATEW_MMDD),100))/100
day=mod(DATEW_MMDD,100)

duplicate/o DATEW_MMDD  timewave
timewave=nan

timewave=date2secs(year,month,day)+(((hour)*3600)+(minute)*60+second)

SetScale/P x 0,1,"dat", timewave;DelayUpdate
SetScale d 0,0,"dat", timewave
```

```
KillWaves/Z hour,minute,second,year,month,day


End
//******************************************************************************
Macro MakeTOTSplots()

MakeTimewave()

B_WS_WD_plot()
B_neph_parms_plot()
B_neph_plot()
B_flightpath_plot()
B_altitude_plot()
B_SO2_plot()
B_ozone_plot()
B_nitrogen_plot()
B_smth_nitrogen_plot()
B_CO_plot()

End


//******************************************************************************
// THIS FUNCTION CONVERTS THE BAYLOR STUDY FLAGS TO THEIR NARSTO
EQUIVALENTS

function Convert2Narsto(qcwave)
wave/t qcwave
variable x=0,n=numpnts(qcwave)

do
		if (cmpstr(qcwave[x],"0")==0)

			qcwave[x]="V0"
		else
			if(cmpstr(qcwave[x],"6")==0)
				qcwave[x]="M2"
			else
				if(cmpstr(qcwave[x],"7")==0)
					qcwave[x]="V6"
				else
					if(cmpstr(qcwave[x],"8")==0)
						qcwave[x]="M2"
					else
```

```
                        if(cmpstr(qcwave[x],"9")==0)
                            qcwave[x]="M1"
                        endif
                    endif
                endif
            endif
        endif
        x+=1

    while (x<n)

end

//****************************************************************************
Macro PowerSpectrum(w)
string w
Prompt w "data wave:",popup WaveList("*",";","")

duplicate/o $w $(w+"x")

RemoveNaNs($(w+"x"))
psd(w+"x",2,2)

killwaves $(w+"x")

end

//****************************************************************************
**************
//This macro calculates the water mixing ratio using measured dewpoint and temperature
//macro CalcWater_to()

silent(1)

duplicate/o tat_degC a h2o ph2o ph2odpt t_k rh_calc  a_dpt dpt_k corr_temp

corr_temp=(.96*(temp_degC))-2.066

interpolatewave(t_k,corr_temp)
interpolatewave(dpt_k,dewpoint_degc)

dpt_k+=273.15
a_dpt=1-(373.15/dpt_k)
t_k+=273.15
a=1-(373.15/t_k)
ph2o=1013*exp((13.3185*a)-(1.9760*(a^2))-(0.6445*(a^3))-(0.1299*(a^4)))
```

```
ph2odpt=1013*exp((13.3185*a_dpt)-(1.9760*(a_dpt^2))-(0.6445*(a_dpt^3))-
(0.1299*(a_dpt^4)))
rh_calc=(ph2odpt/ph2o)*100

h2o=(1e4*rh_calc*(ph2o/pres_mb))/1e3



end

//****************************************************************************
//This macro performs the water correction for the chemiluminescent instruments.  The
//correction is based on calculated water vapor mixing ratio (from calcwater_TO).  The
//correction is 0.4%/ppth water.

macro water_correction()

silent 1
duplicate/o fastO3_ppbv fasto3_ppbv_cor
duplicate/o no_ppbv no_ppbv_cor
duplicate/o no2_ppbv no2_ppbv_cor
duplicate/o noy_ppbv noy_ppbv_cor
duplicate/o noystar_ppbv noystar_ppbv_cor

fasto3_ppbv_cor = FastO3_ppbv+(FastO3_ppbv*(.004*h2o))
no_ppbv_cor = no_ppbv+(no_ppbv*(.004*h2o))
no2_ppbv_cor = no2_ppbv+(no2_ppbv*(.004*h2o))
noy_ppbv_cor = noy_ppbv+(noy_ppbv*(.004*h2o))
noystar_ppbv_cor = noystar_ppbv+(noystar_ppbv*(.004*h2o))


end

//****************************************************************************
macro Generate_AvgData()

silent 1

zscoreCO()

makestartstopwave(5)
make/o/n=(numpnts(starttime)) fasto3_ppbv_5s
make/o/n=(numpnts(timewave)) fasto3_ppbv_5sx
DoAveragOnlyUsingStartStop(timewave, o3_smooth, fasto3_ppbv_5s, starttime, stoptime)
expandit(meantime, fasto3_ppbv_5s, timewave, fasto3_ppbv_5sx)
```

```
make/o/n=(numpnts(starttime)) noy_ppbv_5s
make/o/n=(numpnts(timewave)) noy_ppbv_5sx
DoAveragOnlyUsingStartStop(timewave, noy_smooth, noy_ppbv_5s, starttime, stoptime)
expandit(meantime, noy_ppbv_5s, timewave, noy_ppbv_5sx)

make/o/n=(numpnts(starttime)) noystar_ppbv_5s
make/o/n=(numpnts(timewave)) noystar_ppbv_5sx
DoAveragOnlyUsingStartStop(timewave, noystar_smooth, noystar_ppbv_5s, starttime, stoptime)
expandit(meantime, noystar_ppbv_5s, timewave, noystar_ppbv_5sx)

make/o/n=(numpnts(starttime)) no_ppbv_5s
make/o/n=(numpnts(timewave)) no_ppbv_5sx
DoAveragOnlyUsingStartStop(timewave, no_smooth, no_ppbv_5s, starttime, stoptime)
expandit(meantime, no_ppbv_5s, timewave, no_ppbv_5sx)

make/o/n=(numpnts(starttime)) no2_ppbv_5s
make/o/n=(numpnts(timewave)) no2_ppbv_5sx
DoAveragOnlyUsingStartStop(timewave, new_no2, no2_ppbv_5s, starttime, stoptime)
expandit(meantime, no2_ppbv_5s, timewave, no2_ppbv_5sx)

make/o/n=(numpnts(starttime)) so2_ppbv_5s
make/o/n=(numpnts(timewave)) so2_ppbv_5sx
DoAveragOnlyUsingStartStop(timewave, so2_ppbv, so2_ppbv_5s, starttime, stoptime)
expandit(meantime, so2_ppbv_5s, timewave, so2_ppbv_5sx)

make/o/n=(numpnts(starttime)) co_ppbv_5s
make/o/n=(numpnts(timewave)) co_ppbv_5sx
DoAveragOnlyUsingStartStop(timewave, co_ppbv, co_ppbv_5s, starttime, stoptime)
expandit(meantime, co_ppbv_5s, timewave, co_ppbv_5sx)

make/o/n=(numpnts(starttime)) altitude_ft_5s
make/o/n=(numpnts(timewave)) altitude_ft_5sx
DoAveragOnlyUsingStartStop(timewave, altitude_ft, altitude_ft_5s, starttime, stoptime)
expandit(meantime, altitude_ft_5s, timewave, altitude_ft_5sx)

make/o/n=(numpnts(starttime)) altitude_m_5s
make/o/n=(numpnts(timewave)) altitude_m_5sx
DoAveragOnlyUsingStartStop(timewave, altitude_m, altitude_m_5s, starttime, stoptime)
expandit(meantime, altitude_m_5s, timewave, altitude_m_5sx)

make/o/n=(numpnts(starttime)) pres_mb_5s
make/o/n=(numpnts(timewave)) pres_mb_5sx
DoAveragOnlyUsingStartStop(timewave, pres_mb, pres_mb_5s, starttime, stoptime)
expandit(meantime, pres_mb_5s, timewave, pres_mb_5sx)

make/o/n=(numpnts(starttime)) dewpoint_degc_5s
```

```
make/o/n=(numpnts(timewave)) dewpoint_degc_5sx
DoAveragOnlyUsingStartStop(timewave, dewpoint_degc, dewpoint_degc_5s, starttime,
stoptime)
expandit(meantime, dewpoint_degc_5s, timewave, dewpoint_degc_5sx)

make/o/n=(numpnts(starttime)) temp_degc_5s
make/o/n=(numpnts(timewave)) temp_degc_5sx
DoAveragOnlyUsingStartStop(timewave, temp_degc, temp_degc_5s, starttime, stoptime)
expandit(meantime, temp_degc_5s, timewave, temp_degc_5sx)

end
//***************************************************************************
macro WriteNewFieldsTO()

string list="",header1=""
variable fnum,x=0,y=0,n=numpnts(timewave)


silent(1)


list+="timewave;"
list+="fasto3_ppbv_5sx;"+"no_ppbv_5sx;"+"no2_ppbv_5sx;"+"noy_ppbv_5sx;"
list+="noystar_ppbv_5sx;"
list+="so2_ppbv_5sx;"+"co_ppbv_5sx"

Newfields2()

Save /B/J/O/P=data/W/F  list as basename+".newdat"


End

//***************************************************************************

//PLOT DEFINITIONS
```

Not included here to save space. The electronic version of these procedures available to Baylor and TNRCC include all of the plot definitions.

```
//***************************************************************************
//Wavemetrics power spectrum macro

#pragma version= 1.1
#pragma rtGlobals=1		// Use modern global access method.
```

```
#include <DSP Window Functions>
#include <BringDestToFront>

// Given a long data wave create a short result wave containing the Power
// Spectral Density (PSD).  For the purposes of this macro, PSD is defined in
// terms of the power per frequency bin width. To get the total power you need
// to integrate. The signal is assumed to be a voltage measurement across a
// 1 ohm resistor.
// The name of the new wave is the name of the source + _psd
// Note: if you don't want the baggage of all the window functions, create your own version
// with your favorite and remove the window parameter (or choose a subset)
//
// Version 1.1, LH 971028
// Changes since 1.0: changed normalization to give results as defined above.

Macro PSD(w,seglen,window)
	string w
	Prompt w "data wave:",popup WaveList("*",";","")
	variable seglen=1
	Prompt seglen,"segment length:",popup "256;512;1024;2048;4096;8192"
	variable window=2
	Prompt window,"Window type:",popup "Square;Hann;Parzen;Welch;Hamming;"
						"BlackmanHarris3;KaiserBessel"
;
	PauseUpdate; silent 1

	variable npsd= 2^(7+seglen)				// number of points in group
(resultant psd wave len= npsd/2+1)
	variable psdOffset= npsd/2					// offset each group by this
amount
	variable psdFirst=0						// start of current
group
	variable nsrc= numpnts($w)
	variable nsegs,winNorm  // count of number of segements and window normalization
factor
	string destw=w+"_psd",srctmp=w+"_tmp"
	string winw=w+"_psdWin"					// window goes here

	if( npsd > nsrc/2 )
		Abort "psd: source wave should be MUCH longer than the segment length"
	endif
	make/o/n=(npsd/2+1) $destw
	make/o/n=(npsd) $srctmp,$winw; $winw= 1
	if( window==1 )
		winNorm= 1
	else
```

```
	if( window==2 )
		Hanning $winw;winNorm=0.372  //  winNorm is avg squared value
	else
		if( window==3 )
			winNorm= Parzen($winw)
		else
			if( window==4 )
				winNorm= Welch($winw)
			else
				if( window==5 )
					winNorm= Hamming($winw)
				else
					if( window==6 )
						winNorm= BlackmanHarris3($winw)
					else
						if( window==7 )
							winNorm= KaiserBessel($winw)
						else
							Abort "unknown window index"
						endif
					endif
				endif
			endif
		endif
	endif
endif

Duplicate/O/R=[0,npsd-1] $w $srctmp; $srctmp *= $winw; fft $srctmp
CopyScales/P $srctmp, $destw
$destw= magsqr($srctmp)
psdFirst= psdOffset
nsegs=1
do
	Duplicate/O/R=[psdFirst,psdFirst+npsd-1] $w $srctmp;   $srctmp *= $winw
	fft $srctmp;   $destw += magsqr($srctmp);   psdFirst += psdOffset; nsegs+=1
while( psdFirst+npsd < nsrc )
winNorm= 2*deltax($w)/(winNorm*nsegs*npsd);  $destw *= winNorm
$destw[0] /= 2

KillWaves $srctmp,$winw
BringDestFront(destw)
if( numpnts($destw) <= 129 )
	Modify mode($destw)=4,marker($destw)=19,msize($destw)=1
else
	Modify mode($destw)=0
	ModifyGraph log=1
```

```
	endif
end


//******************************************************************************
macro makepathsTO()
string/g basename, data_folder, plots_folder



basename=current_file[0,12]

data_folder="C:Projects:STI:Baylor:Data:"
plots_folder="C:Projects:STI:Baylor:Plots:"

newpath/c/o data data_folder
newpath/c/o plots plots_folder

newpath/c/o data data_folder+basename
newpath/c/o plots plots_folder+basename


print data_folder
print plots_folder


end

//****************************************
macro narstoQC()
silent 1

convert2narsto(LAT_QC)
convert2narsto(LON_QC)
convert2narsto(Altitude_ft_QC)
convert2narsto(Altitude_m_QC)
convert2narsto(FastO3_QC)
convert2narsto(NOy_QC)
convert2narsto(NOyStar_QC)
convert2narsto(NO2_QC)
convert2narsto(NO_QC)
convert2narsto(SO2_QC)
convert2narsto(Pres_QC)
convert2narsto(DewPoint__QC)
convert2narsto(SlowO3_QC)
convert2narsto(bsp_QC)
```

```
convert2narsto(Gsp_QC)
convert2narsto(Rsp_QC)
convert2narsto(Bbsp_QC)
convert2narsto(Gbsp_QC)
convert2narsto(Rbsp_QC)
convert2narsto(NephP_QC)
convert2narsto(NephSAM_QC)
convert2narsto(NephInlt_QC)
convert2narsto(NephRH_QC)
convert2narsto(IAS_QC)
convert2narsto(TAS_QC)
convert2narsto(PALT_QC)
convert2narsto(DALT_QC)
convert2narsto(OAT_QC)
convert2narsto(TAT_QC)
convert2narsto(WDIR_QC)
convert2narsto(WSPD_QC)
convert2narsto(HDNG_QC)
convert2narsto(ValveTime_QC)
convert2narsto(CellInd_ascii_QC)
convert2narsto(RHvolts_QC)
convert2narsto(TMPvolts_QC)
convert2narsto(FMvolts_QC)
convert2narsto(VoltDP_QC)
convert2narsto(CellSig_QC)
convert2narsto(CellBase_QC)
convert2narsto(Temp_QC)
convert2narsto(CT_QC)
convert2narsto(CellSigCellBASE_QC)
convert2narsto(CO_QC)
end
//*****************************************************************************

Menu  "Baylor Twin Otter "
"_________________"
	Submenu "TexAQS 2000"
		"ReadTwinOtterFile"
		"MakeTOTSplots"
		"PowerSpectrum"
		"CalcWater_TO"
		"ratio_analysis"
		"water_correction"
		"Generate_AvgData"
		"makepathsTO"
		"WriteNewFieldsTO"
	End
```

```
	Submenu "Baylor 2001"
		"ReadTwinOtterFile2001"
		"ReadTwinOtterFile2001woStat"
		"ReduceTO2001"
	End
"________________"
End
```

```
#pragma rtGlobals=1		// Use modern global access method.


//Option Explicit
//This was programmed by Joshua Begbie of Baylor University (in VB) for use in analyzing the
//air pollution data the Aviation Sciences Department collected in their aircraft.  It is designed to
//take out  measurement errors inherent in the NO2 instrument, and is heavily based on an
//algorithm //provided by the Tennessee Valley Authority.
//10-15-00 Sergio L. Alvarez set NOTimeShift and O3TimeShift to 0.
//10-31-00 Sergio L. Alvarez set O3Time ande NOTime to 2.2 seconds.
//07-20-01 Joshua Begbie changed column location constants to account for data layout changes
//Translation from the VB to Igor Pro by Martin Buhr (STI) August 2001.

Macro ReduceNO2()
//This is a list of constants used throughout the program
	variable n=numpnts(timewave),x=0
	variable/g NOi=0 //measured NO
	variable/g O3i=0 //measured ozone
	variable/g NO2i=0 //measured NO2
   variable/g k=0 // reaction rate constant calculated as  k = 0.0000000000018 * Exp(-1370 /
(OAT)) * 17500000000
   variable/g NOa=0 //calculated NO value
   variable/g O3a=0// calculated O3 value
   variable/g DelNO=0//The change in NO looking at the decay in the instrument tubing
   variable/g NOb=0//NOb is the calculated NO value accounting for decay through inst. tubing
   variable/g O3b=0//O3b is the calculated O3 value accounting for decay through inst. tubing
   variable/g NOc=0//NOc
   variable/g O3c=0//O3c
   variable/g NOd=0//NOd is the calculated NO value accounting for decay after the photocell
   variable/g O3d=0//O3d is the calculated O3 value accounting for decay after the photocell
   variable/g NO2trial=0//NO2trial is the value of ambient NO2 to be used in an interation
   variable/g DELT=0//Defines the iteration step size for the convergence loop
   variable/g NOplug=0//NO concentration in volume as the gas travels through the cell
   variable/g O3plug=0//O3 concentration in volume as the gas travels through the cell
   variable/g NO2plug=0//NO2 concentration in volume as the gas travels through the cell
   variable/g LoopCounter=0// the counter for the convergence loop
   variable I=0//an iteration loop counter
   variable/g NO2err=0//the difference of the estimated and instrument's value of NO2
   variable/g PreTime= 2.2
	variable/g CellTime= 15.5
	variable/g PostTime= 0.41
	variable/g O3Time= 2.2
	variable/g NOTime= 2.2
	variable/g NOTimeShift=0   //Time shift lead for the NO instrument over the NO2
	variable/g O3TimeShift=0   //Time shift lead for the O3 instrument over the NO2
	variable/g JVal=.09
```

```
//prompt JVal, "What is the j value for the flight?"

silent 1

//Sub NO2Calibrate2()
duplicate/o noy_ppbv_cor noy_smooth
duplicate/o NOy_QC NOy_smooth_QC
duplicate/o no_ppbv_cor no_smooth
duplicate/o no_QC NOy_smooth_QC
duplicate/o noystar_ppbv_cor noystar_smooth
duplicate/o noystar_QC noystar_smooth_QC
duplicate/o fasto3_ppbv_cor o3_smooth
duplicate/o fasto3_QC fasto3_smooth_QC
duplicate/o no2_ppbv_cor no2_raw
duplicate/o no2_QC no2_smooth_QC
duplicate/o no2_raw new_no2
duplicate/o no_ppbv_cor no_x
duplicate/o fasto3_ppbv_cor o3_x
duplicate/o no2_raw converged solved
converged=0
solved=0

//This section contains the data smoothing algorithms (smooth_no and smooth_o3 are functions
//shown at the end of the macro)
//(all functions were provided by Martin Buhr of Sonoma Technology)

smooth_no(noy_smooth,noy_ppbv_cor,5)
smooth_no(noystar_smooth,noystar_ppbv_cor,5)
smooth_no(no_smooth,no_ppbv_cor,6)
smooth_o3(o3_smooth,fasto3_ppbv_cor,2)

//Generate temp data for every observation
duplicate/o tat_degC temp_k
interpolatewave(temp_k,tat_degc)
temp_k+=273.15

//Timeshift the NO2_raw signal
insertpoints n,3,no2_raw
deletepoints 0,3,no2_raw

do

	NOi = no_smooth[x]
	O3i = o3_smooth[x]
	NO2i = no2_raw[x]
```

```
            //calculate the k value to be used for the O3 NO back reaction in the cell
            k = 0.0000000000018 * Exp(-1370 / (temp_k[x])) * 17500000000

           //calculate ambient NO & O3 based on instrument measurement & residence time to instr.

             O3a = O3i / Exp(-k * O3Time * NOi)
            NOa = NOi / Exp(-k * NOTime * O3a)

             o3_x[x] = O3a //write corrected O3 value to file
             no_x[x] = NOa //write corrected NO value to file

            NO2trial = NO2i - NOi

            DelNO = (k * O3a * NOa) * PreTime
            NOb = NOa - DelNO
            O3b = O3a - DelNO

            LoopCounter = 0
            DELT = 0.1


                  calcPlug(jval)


//the outcome of this is an estimate for NO2a which is now updated in the chart

            new_no2[x] = NO2trial

        x+=1

while (x<n)

end

//****************************************************************************

function smooth_no(w1,w2,s)
wave/d w1,w2
variable s
variable x=0,n=numpnts(w2)
w1=0
do
```

```
		w1[x]+=(w2[x]*0.0485+w2[x+1]*0.06+w2[x+2]*0.088)
		w1[x]+=(w2[x+3]*0.115+w2[x+4]*0.129+w2[x+5]*0.129)
		w1[x]+=(w2[x+6]*0.118+w2[x+7]*0.0994+w2[x+8]*0.0778)
		w1[x]+=(w2[x+9]*0.0581+w2[x+10]*0.0418+w2[x+11]*0.0275)
		w1[x]+=(w2[x+12]*0.0157705)

	x+=1

while (x<n)

insertpoints 0,s,w1
w1[0,s]=nan
deletepoints n,s,w1

end

//*************************************************************************
function smooth_o3(w1,w2,s)
wave/d w1,w2
variable s
variable x=0,n=numpnts(w2)
w1=0
do

		w1[x]+=(w2(x)*0.121853+(w2(x+1)*0.133431+w2(x+2)*0.135584))
		w1[x]+=(w2(x+3)*0.116727+w2(x+4)*0.102509+w2(x+5)*0.0900861+w2(x+6)*0.0678
155)
		w1[x]+=(w2(x+7)*0.0373737+w2(x+8)*0.0224105+w2(x+9)*0.0292239+w2(x+10)*0.0
359615)
		w1[x]+=((w2(x+11)*0.0338168+w2(x+12)*0.0292643+w2(x+13)*0.0266016+w2(x+14)
*0.0173418))

	x+=1

while (x<n)

insertpoints 0,s,w1
w1[0,s]=nan
deletepoints numpnts(w2),s,w1

end

//**********************************************************************
function CalcPlug(jval)
variable jval
```

```
wave converged,solved,new_no2,no2_raw
variable
i,celltime,delt,delno,no2plug,k,o3plug,noplug,loopcounter,noa,o3b,no2trial,noc,o3c,nod,o3d,post
time,no2err,no2i


        Do
          LoopCounter = LoopCounter + 1
          NOplug = NOa
          O3plug = O3b
          NO2plug = NO2trial

          //perform stepwise integration for photo cell
          //plug refers to the concentration in volume as it travels through the cell
          For(i=0;i<celltime;i+=delt)
            DelNO = ((JVal * NO2plug) - (k * O3plug * NOplug)) * DELT
             NOplug = NOplug + DelNO
              NO2plug = NO2plug - DelNO
              O3plug = O3plug + DelNO
          endfor

          //the plug is now through the photocell.
          //the last value is the estimated value for step C (output from the cell)
          NOc = NOplug
          O3c = O3plug

          //now calculate the decay of NO after the photocell to the instrument
          NOd = NOc * Exp(-k * PostTime * O3c)
          O3d = O3c * Exp(-k * PostTime * NOc)

          //does the estimate for NO at the instrument agree with the instrument value
          NO2err = NO2i - NOd

          //check to see if the error is within range or the counter is too high
          If (Abs(NO2err) < 0.01)
             Converged[x] = 1
             solved[x]=1
                 ElseIf (LoopCounter > 100)
                           Converged[x] = 1
                           Solved[x]= 0
          Else
             NO2trial = NO2err / 2 + NO2trial
          EndIf
```

```
		while (converged[x]==0)

		//the outcome of this is an estimate for NO2a which is now updated in the chart
	new_no2[x] = NO2trial
end
```

APPENDIX B

POSTER TITLED "DATA QUALITY AND UNCERTAINTY ANALYSIS FOR THE BAYLOR UNIVERSITY TRACE GAS OBSERVATIONS COLLECTED DURING THE TexAQS 2000 STUDY"

PRESENTED AT THE TexAQS 2000 DATA MEETING IN AUSTIN, TEXAS, AUGUST 4-9, 2001

Description and Uncertainty Analysis of the Baylor University Aircraft Trace Gas Observations Collected during the TexAQS 2000 study

Martin Buhr, Sonoma Technology, Inc., Petaluma, CA

Introduction

The goal of this work was to improve the quality and confidence level of the Baylor University Twin Otter data set that will be submitted as part of the TexAQS 2000 air quality study and to prepare a self-consistent data set for the flights conducted during TexAQS 2000 for subsequent data analysis. The work focused on the data collected for NO, NO_2, NO_y, and NO_y*, ozone, CO, and SO_2. Data quality was improved by identifying an appropriate averaging interval for the data. The confidence level of the data was established through creation of an uncertainty budget for the measurements

Descriptive Statistics and Analysis

Concentration distribution

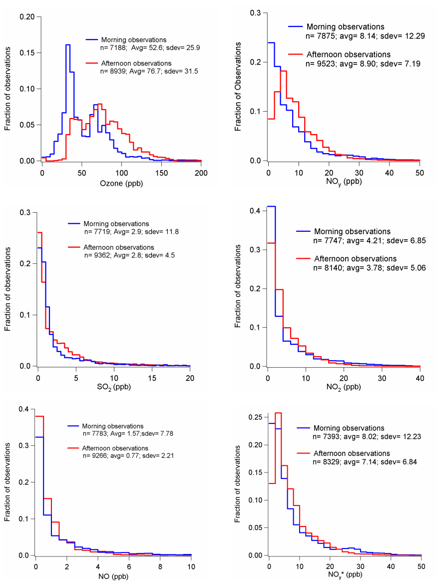

Figure 1. Histograms for the trace gas measurements collected during the study. Assuming normal or log-normal distributions it is clear that the LOD of all of the measurements except ozone are not adequate to describe the complete distribution of concentrations present. However, with the possible exception of NO, the mode of the distribution is probably represented. The difference between the morning and afternoon observations is consistent with both fresh and aged emissions in the morning and greater photochemical transformation in the afternoon.

Frequency response

The response speed of all of the chemical and physical sensors utilized during the study was assessed through analysis of power spectra of the data collected. This information was used to arrive at an optimal data reporting rate for all of the measurements. Based on this analysis the trace gas measurements were averaged over a period of 10 seconds.

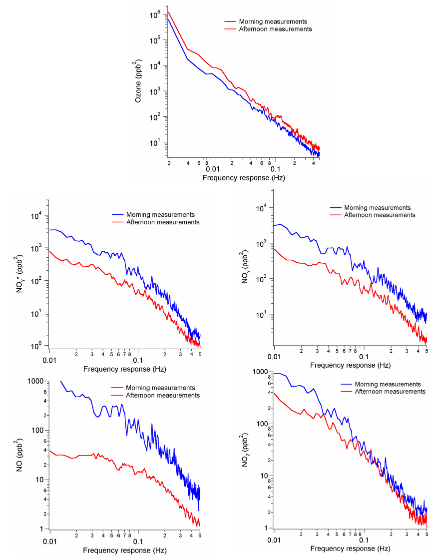

Figure 2. Example power spectra for ozone and the reactive nitrogen species measurements collected during the study. Ozone showed good response speed up to 0.5 Hz. The response speed of the reactive nitrogen measurements was consistently above 0.3 Hz. NO_y and NO_y* showed somewhat slower response in the morning measurements, indicating possible retention of HNO_3 on the inlet systems.

Uncertainty Budget

An uncertainty budget for each of the trace gas measurements was estimated assuming a normal distribution of errors. The categories of error considered are shown in the following Table.

Parameter	Calibration standard (note 1)	Conversion efficiency (note 2)	Repeatability (note 3)	Baseline (note 4)	Combined uncertainty (note 5)
UV Ozone (slow)	5%	N/A	6%	1 ppb	8% + 1 ppb
Chemluminescent Ozone (fast)	5%	N/A	15%	2 ppb	16% + 2 ppb
NO_y	6%	20%	3%	4 ppb	21% + 4 ppb
NO_yStar	6%	3%	3%	6 ppb	7 % + 6 ppb
NO_2	6%	8%	4%	3 ppb	11% + 3 ppb
NO	4%	N/A	3%	1 ppb	5% + 1 ppb
SO_2	4%	N/A	9%	0.3 ppb	10% + 0.3 ppb
CO	4%	N/A	127%	48 ppb	130% + 48 ppb

Notes:

1. Calibration standard. Uncertainty on the calibration standard includes the uncertainty on the gas mixture and dilution. For ozone (also the NO_2 calibrations produced using ozone) the uncertainty reflect the variation in the ozone source.
2. Conversion efficiency. For NO_2 and NO_y* the uncertainty in conversion efficiency is estimated from repeated calibrations. For NO_y an additional uncertainty was estimated since HNO3 conversion efficiency was not determined.
3. Repeatability. This uncertainty was estimated from the standard deviation of the slopes from approximately 65 calibrations conducted during the study.
4. Baseline. The uncertainty in the baseline, or zero level of the measurements was estimated from the standard deviation of the zero level determinations (synthetic air) conducted during the study. Although the measurements were corrected from the zero level, this number reflects the expected variability of that level during ambient measurements.
5. Combined uncertainty. The combined uncertainty was estimated through propagation of the above uncertainties as $((d_1)^2 + (d_2)^2 + (d_n)^2)^{1/2}$.

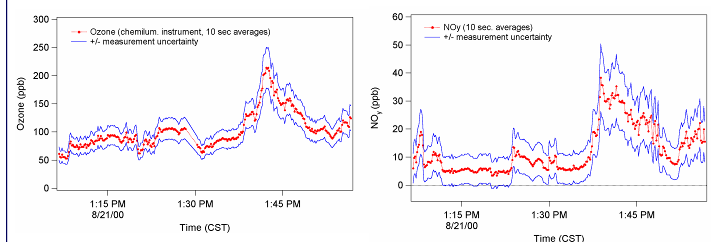

Figure 3. Example time series of 10 second average ozone and NO_y data with 1σ uncertainty limits.

Summary

•The trace gas instrumentation operated on the Baylor University Twin Otter had adequate sensitivity and response speed to characterize most of the air parcels observed during the TexAQS 2000 study.
•With the exception of the CO measurement, which is still under evaluation, the uncertainty associated with each measurement is within reason
•Current work is aimed at decreasing the measurement uncertainty through implementation of automatic, ambient air, zero level determinations.

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Sonoma Technology, Inc.