

NOAA-ESRL

GLOBAL MONITORING LABROATORY

Surface Ozone Handbook

Version 1.0 | Revised 2/15/2021

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Document Revision Table

Revision No.	Revision Date	Notes
0	2015	Original Document
1.0	2/15/2021	Updated for new 49iQ instrument; formatting changes; new contact information; changes to Data collection methodology

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1) Introduction

This document has been written and designed for individuals that are responsible for maintenance and data collection of surface ozone measurements from Thermo Scientific Ozone monitors supported by the National Oceanic and Atmospheric Administration/Earth Systems Research Laboratory/Global Monitoring Laboratory Surface Ozone Monitoring Network.

Surface Ozone or Ground-Level Ozone is the primary component of photochemical smog and is harmful to public health and ecosystem functioning. As a secondary pollutant, it is formed by the reaction of Nitrogen Oxides (NOx) and Volatile Organic Carbons (VOC's) in the presence of UV radiation. Surface level ozone is monitored through the Global Monitoring Division at 15 different locations. Since the Clean Air Act of 1970, the US Environmental Protection Agency has established ozone as a health and environmental concern. Therefore, regulatory actions and standards were established for ground level ozone. As a critical atmospheric species which regulates the oxidation capacity and photochemistry of the troposphere, ozone is monitored as the third most important contributor to greenhouse radiative forcing. NOAA/ESRL/GML is responsible for maintaining accurate data with minimal loss of data for report for scientific understanding of this pollutant.

2) Theory of Operation

All ozone monitors in the NOAA/ESRL/GMD Surface Ozone monitoring network are Thermo-Scientific 49 series ozone monitors. This ozone monitor uses the Beer-Lambert Law measuring the degree to which UV light is absorbed at 254 nm and relating this to the ozone Concentration. The sample air is pulled into the instrument through a Teflon inlet tube and is split into two streams. Stream 1 is scrubbed of ozone and becomes the reference air sample. Stream 2 is unaltered sample air. The UV light of each stream is measured and the average concentration is displayed on the instrument front Panel.

3) Instrument Specifications

Model	Link to manual
49C	ftp://aftp.cmdl.noaa.gov/ozwv/SurfaceOzone/QA%20Docs/Model%2049C.pdf
49i	https://www.thermofisher.com/order/catalog/product/49I#/49I
49iQ	https://www.thermofisher.com/order/catalog/product/49IQ#/49IQ

	49C	49i	49iQ
Zero Noise	0.5 ppb	0.25 ppb	0.25ppb
Response Time	20 seconds	20 seconds	20 seconds
Precision	1 ppb	1 ppb	Not shown
Linearity	± 1% Full-scale	± 1% Full-scale	± 1% Full-scale
Sample Flow Rate	1-3 LPM	1-3 LPM	1-3 LPM
Operating Temperature	20-30 degrees C	0-45 degrees C	0-45 degrees C
	150 Watts	150 Watts	200 Watts
Power Requirements	90-250 VAC@50/60Hz	100-240 VAC@50/60Hz	100-240 VAC@50/60Hz
Physical Properties	16.75" x 8.62" x 23" 35 lbs	16.75" x 8.62" x 23" 35 lbs	16.75" × 8.72" × 24" 36 lbs
Ranges	0-200 ppm	0-200 ppm	0-200 ppm

49C Interface:

With Zero/Cal knob



Button	Action from Main Screen	Action from Menu screen
Run	Toggles between Sample, Level 1	Takes you back to Main Screen
	and 2, and Zero	
Menu	Enters the main Menu	Go back
Enter	Toggles between Remote and	Select item / Save configuration changes
	Local mode	
Help	Shows helpful tips	Shows helpful tips

Without knob

49i interface:



Button	Action from Main Screen	Action from Menu screen
Run	Toggles between Sample, Level 1	Takes you back to Main Screen
	and 2, and Zero	
Menu	Enters the main Menu	Go back
Enter	nothing	Select item / Save configuration changes
Help	Shows helpful tips	Shows helpful tips

Calibration Check Menu Home Screen (dual or auto range mode) iQSeries ? Title Bar 49iQ Analyzer Sample Calibration User Interface -O₃ Low 9.3 ppb Data Settings 10/06/17 13:11:23 thermo scientific \bigcap Status Bar -• Back Status Lock Favorites

49iQ interface:

To view ozone real-time graph:

From the home screen, select "Data" then "View Data Log (Last hour)" Then touch "Graph"

Time Stamp	Concentration (ppb or ug/m3)	з	4	5	6	
	Graph					
10/14/2017 15:19:00	-3.90683					
10/14/2017 15:18:00	-3.88464					
10/14/2017 15:17:00	-3.8487					
10/14/2017 15:16:00	-3.70784					
10/14/2017 15:15:00	-3.4842					
10/14/2017 15:14:00	-3.44236					_
10/14/2017 15:13:00	-3.40246					
10/14/2017 15:12:00	-3.34265					

4) Installation

Ozone is the product of complex photochemical reactions in the atmosphere and therefore is not emitted directly into the air. Ozone can form, accumulate, and disperse over a large area. High ozone episodes are often related to a complex blend of hydrocarbons, high solar radiation, high temperatures, and low wind speeds. Monitoring instrumentation must be kept in a dry, clean, and temperature controlled space with power and inlet lines accessible for maintenance.

Note: Only connect fittings of the same material. (ie. Stainless steel to stainless steel or Kynar to Kynar or Teflon to Teflon). For Kynar, Teflon, or other plastics, tighten to "Hand tight" - Do not use a wrench. For metal fittings don't tighten more than 1/4 turn past hand tight.

Installation Requirements:

120 VAC power source AC or Heat to maintain relatively stable temperatures Operator accessibility to front, back, and inlet lines of instrument

Installation Parts required:

Instrument External Pump Charcoal Filter Desiccant (tropical sites) Instruction Manuel Sample line particulate Filter (aka "Savillex filter") NULL serial Cable UPS (universal power supply) if possible

Inlet Location:

Unrestricted flow through inlet tube Air flow around the inlet Vertical distance from ground (3-15 meters) and support structures (1 meter)

Setup Instructions:





Once instrument location and inlet lines have been selected, the following procedure will allow for complete set-up of the instrument.

- 1. Locate and feed inlet line to sampling instrument location
- 2. Ensure that orange filter assembly is attached to inlet line or a bell filter outside to remove particulates from sample air. Arrow on orange filter shows the direction air will be flowing into the instrument.
- 3. Connect the sample line to the SAMPLE bulkhead on the instrument.
- 4. Connect the EXHAUST Bulkhead to a vent exhaust line
- 5. Connect the zero scrubber air to the ZERO AIR bulkhead
- 6. Connect instrument to computer with a Null cable or USB cord
- 7. Turn on instrument and allow to warm up for 20 minutes

5) Instrument Alarms and Notifications:

TEI Ozone 49 instruments monitor the conditions and status of the instrument and will report an alarm if a problem has been detected.

49C/i Alarms:

To access the alarms-enter the main menu and select alarms. There will be a list of alarm types and status for each (OK, LOW, HIGH)

49iQ Alarms:

On the main screen, the green check mark will be replaced with a Red triangle when there is an alarm. Touch the Red triangle to view alarms.

Alarm Type	Description	Standard Limits	Notes/Fixes
O3 lamp temperature (49i)	Ozonator lamp temp	65-75 Degrees C	Bad MOLEX connection Defective lamp heater
Lamp temperature	Lamp Temperature	50-60 Degrees C	Bad MOLEX connection Defective Lamp heater
Bench Temperature	Instrument Temperature	5-50 Degrees C	Bad MOLEX connection Faulty Fan High room temperature
Pressure	Pressure of Instrument	400-1000 mmHg	Tear in diaphragm Check for tubing leaks
Flow (49C and 49i)	Flow of sample air into cell A or B	0.4 – 0.9 LPM	1 low: Check for capillary blockage Both low: Pump or pump diaphragm bad
Flow (49iQ)	Flow of sample air into internal pump	1.2 – 1.7 LPM	
Intensity (A/B)	Lamp intensity on each cell A or B	65000-120000 Hz	Check Gain adjustment and lamp intensity Dirty Cells
	Noise (Fully warmed lamp)	4Hz	
O3 Concentration	Current O3	0-120 ppb (ambient)	

FOR NOAA STATION TECHNICIANS AND SCIENTISTS: IF AN ALARM IS DETECTED, PLEASE CONTACT:

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6) Calibration Checks (aka QC checks)

Station calibrations checks are checks for quality control to compare the span of ozone measured by the instrument. Station calibrations are done weekly, bi-weekly, or monthly depending on station location and personnel. The station calibrations are manually performed monitoring ozone at three concentration levels: zero, level 1 (35ppb), and level 2 (75ppb).

Calibration check procedure for 49C and 49i instruments

- Turn on external pump Ensure that pump/charcoal scrubber is connected to the zero air on the back of the TEI
- 2) (For 49C "knob style" instruments): Press "Enter" so the screen reads "Local" in the lower right. Turn the knob to 'CAL'
- 3) Press the RUN button to initiate the 1st measurement: LEVEL 1. Allow level 1 to run until the ozone readings stabilize (Approximately 12-15min although can be

longer in some situations).

- 4) Press the RUN button to start the 2nd measurement: LEVEL 2. Allow level 2 to run ozone readings stabilize (Approximately 12-15 min).
- 5) Press the RUN button to start the 3rd measurement: ZERO. (For 49C "knob style" instruments, turn the knob to "Zero". Allow zero to run until the ozone readings stabilize (Approximately 12-15min although can be longer in some situations).
- 6) Press the RUN button until the SAMPLE mode is displayed.
- 7) (For 49C "knob style"): Press Enter so the screen reads "Remote" in the lower right. Turn the knob to "CAL"
- 8) Turn off external pump
- 9) Ensure that instrument is reading sample air.

Calibration Check procedure for 49iQ instruments:

- Turn on external pump Ensure that pump/charcoal scrubber is connected to the zero air on the back of the TEI
- 2) Touch the "Sample" in the upper left



- 3) Choose 'Level 1' Let it run for 12-15 minutes and record results
- 4) Touch 'Level 1' (sample spot as sample in figure above) and choose 'level2' Let it run for 12-15 minutes and record results
- 5) Touch 'level2' (sample spot as sample in figure above) and choose 'zero' Let it run for 12-15 minutes and record results
- 6) Finally, Choose "sample" and ensure that the analyzer is now reading ambient air.
- 7) Turn off external pump.

7) Data Collection

Most surface ozone sites collect data through the NOAA Global Monitoring Laboratory Aerosol Group 'CPD3' software. However, there are times when manual data downloads may be needed

(for example if there is a network outage or if the site does not have the CPD software)

CPD3 Aero system

The Live-CPD3 software is developed by the NOAA Global Monitoring Laboratory Aerosol Group and is used for data collection and processing. The TEI ozone instrument at most stations is connected directly to a laptop suited for CPD running on a Linux operating system. The program allows for data reports to be sent to the PI daily and data to be collected automatically – without need for manual data download from the instrument. The ozone instrument is connected to the aero computer either via RS-232 / NULL DB9 cable connected directly to the laptop or over TCP/IP over the Ethernet network.

Further information on CPD software can be found here: https://esrl.noaa.gov/gmd/aero/sw.html

The User manual for CPD3 edited for the surface ozone network can be found here:

ftp://aftp.cmdl.noaa.gov/ozwv/SurfaceOzone/QA_Docs/Using_CPX3_Ozone

Download Data from a 49C or 49i instrument Thermo iPort

- 1) Open iPort
- 2) 49C: Click on the drop-down menu "Comm" and click "Connect":49i: Click on "Instrument" and then "TCP Connect" then "Connect"



- 3) Select "Yes" to connect to the instrument"
- 4) The instrument window will open
- 5) From the tool bar click the icon for "Load records"
- 6) Download Short Records Select the following: Short Records, 4000 records back and check "Save to file" Rename the file with station identifier and .src.
- 7) Click OK to load records.
- Download Long Records.
 Select "Long Records, 1000 records back, and click "Save to file" Rename the file with station identifier and .lrc
- Both files are typically located in C:\Thermo\iPort However, you may specify a different path in the "Save to file" Box.

For example:

10) Download data to FTP Server for transfer to PI for analysis.

Download Data from a 49iQ instrument using Thermo ePort

- 1) Open Thermo ePort
- 2) Click the 49i instrument on the left side of the window
- 3) Click on Download Setup
- 4) Click Next
- 5) Choose "from last download or selected date and time" and click "next"
- 6) Select a location that is convenient for you (I suggest to click "Browse" and select the desktop) and click "Next" then "Finish"
- 7) Click on the Download Data button
- 8) Select "Begin Download"
- 9) When the Download if complete it will display a "Download Complete" Message.

8) Data Quality

Extensive data quality checks are completed at NOAA-GMD on a monthly basis. However, Technicians and station personnel can assist in ensuring complete, usable data is sent to the NOAA servers. Data quality checks are essential for monitoring the condition and status of the instrument.

Data Quality Indicator	Acceptable Limits	Notes
Instrument Alarms Activated	Alarm Dependent	Notify PI of alarm message
		Notify PI if drift is out of the 10%
Station Calibration Check	1-4 times per month ± 10%	range
NIST Calibration	1 / 4 years	Performed at NOAA-Boulder
	1 hour average data – 90% of	Instrument problems need
Completeness	measurements	documentation

Full Quality Assurance procedures can be found in the Surface Ozone Quality Assurance Project Plan (QAPP) here: <u>ftp://aftp.cmdl.noaa.gov/ozwv/SurfaceOzone/QA%20Docs/</u>

9) Routine Procedures

Daily Checks:

Some stations perform daily instrument checks. This is not required for all stations-If your station performs daily checks, please do the following

- Record Diagnostics (49C, 49i):
 - 1) From the menu of the TEI
 - 2) Press the Arrow down to Diagnostics
 - Under the following menus, record the following diagnostics: Temps: Bench, Bench Lamp, O3 Lamp Pressure: Pressure (Photometer Pressure) Flows: Cells A and B Intensities: Cells A and B
- Record Diagnostics (49iQ)
 - 1) Touch "settings" on the main screen
 - 2) Touch "Health Check"
 - 3) Touch "Status and Alarms"
 - Under the following menus you can find the diagnostic information: Photometer Bench: Photometer Pressure, Flow, Bench Temperature, Intensities Ozonator: Lamp Temperature Flow and Pressure: Flow, Photometer Pressure, Pump Pressure, Module Temperature
- Check for instrument alarms
- Compare instrument readings to climatology. For most sites, ambient ozone under normal conditions should be in the range of 20-70ppb.
- Note any unusual activity that may impact data (e.g. vehicle idling under inlet, power outage, liquid water, dirt, or bugs in the sample line, etc.).

Weekly or Bi- weekly Level Checks:

The frequency of these checks are site dependent. They can be completed anywhere from once per month to once per week. The more frequent the better, but the PI at each site will determine the actual frequency based on local logistics.

- Complete a Calibration check as outlined in Section 6.
- Perform the tasks outlined in Daily Checks.
- Check the time. If the internal clock is off by more than 2min, change the clock so that it matches within one minute of UTC.
- Check the foam fan filter on the back of the instrument. If it is excessively dirty, take if off and clean it using a vacuum or compressed air canister. If ripped or old, replace it.

Monthly Checks

- Check External Filter status- if visible dirt is on the filter prior to specified change time, change the filter and note that filter was dirty prior to routine change.
- Check inlet status
- No bends or breaks in the line

- No evidence of water in the line
- Snug connection with Swagelok on filter assembly and to instrument

Startup Procedure:

• This is an easy one: simply turn on the instrument.

Shutdown Procedure:

• Also easy: simply turn it off.

Calibration and maintenance:

• Once every three years, the analyzer should be sent back to Boulder, CO for calibration against a NIST standards and have maintenance performed.

10) References

- McClure-Begley, Audra and Irina Petropavlovskikh "ESRL Global Monitoring Laboratory Ozone and Water Vapor Division." Web 1 Feb 2021 http://www.esrl.noaa.gov/gmd/ozwv/surfoz.
- Oltmans, S.J., O. Uchino, C.P. Meyer, E.-G. Brunke, I.E. Galbally, H. Levy, J. M. Harris, H.E. Scheel, A.S. Lefohn, V. Mohnen, J.B. Kerr, H. Claude, D. W. Tarasick, F.J. Schmidlin, E. Cuevas, D.S. Chadwick, B.J. Johnson, and J. A. Lathrop. "Trends of ozone in the troposphere." *Geophysical Research Letters* 25.2 (1998): 139. Print.

11) Data citation and Acknowledgement

The scientists and PI's of the Surface ozone network provide data open and free from the Laboratory ftp:

ftp:/aftp.cmdl.noaa.gov/ozwv/SurfaceOzone/

Please ensure that data is cited as follows (adjustments to formatting are common and not a problem as long as the required information is included in the citation used).

McClure-Begley, A., Petropavlovskikh, I., Effertz, P., (2021) NOAA Global Monitoring Laboratory Surface Ozone Network. *Station name, Time start-Time end.* National Oceanic and Atmospheric Administration, Earth System Research Laboratory Global Monitoring Laboratory. Boulder, CO. *Date Accessed* <u>http://dx.doi.org/10.7289/V57P8WBF</u>

insert station name and dates of data used as well as date data was accessed

We ask that all users contact Audra McClure or Peter Effertz regarding data used in publications for information regarding citation and acknowledgment.

Appendix A – Installation and configuration of iPort and ePort software

iPort and ePort will only run on Windows computers. Installation files can be found here: iport: <u>https://assets.thermofisher.com/TFS-Assets/CAD/Software-Updates/iPort%20v1.4.2.zip</u> eport: <u>https://assets.thermofisher.com/TFS-Assets/CAD/Software-Updates/ePort_Setup_4_0_0.zip</u>

Download and install the software leaving all configuration options as default is preferred.

Configure iport for serial (RS-232) connections (typically with 49C):

- 1) Click on "File" in the toolbar and select "Preferences"
- 2) Under "Ethernet" ensure that both "ESC 8832" and "Direct TCP/IP" is unchecked



- 3) Click "OK"
- 4) Click on "Comm" in the Tool bar and click "Connect"
- 5) Click on "Edit" in the new window that opens
- 6) Change the Com port to the correct port the instrument is connected to.
- 7) Leave the settings at 9600, 8-1-N, No Handshake (unless instrument is configured differently).
- 8) Change Poling Conifg to just 49.

File Comm Ir	ntific Instrument Window Help	
Console Initializing E Done. Initializing E Done. Preferences	Communications Settings × Location Thermo Scientific OK Com Baud Rate Len Stop Parity Handshake Cancel 1 • 9600 • 8 • 1 • N • None • Phone Number Enable Modem Autodial 1-508-553-6995 Polling Config Autopoll 49	
	Connect to selected location?	

9) Click "Yes"

Configure iPort for TCP/IP connections (Typically for 49i instruments)

1) Open Click on "File" in the toolbar and select "Preferences"

2) Under "Ethernet" ensure that "ESC 8832" is unchecked and "Direct TCP/IP" is checked

) Concole I Treferences		1	×
General General Automatic Connect Hangup Console Log Enable ♦ Create Automatic Hangup Console Log Enable ♦ Create Automatic Hangup Console Log © Hangup Console Log © Hangup Console Log © Hangup Console Log © Enable ♦ Create Papeur Horsages ♥ Warning ♥ Console ♥ Pop Up Report Traffic © Modem © Instrumer	Modem Command Prefix AT Command Suffix I3 ASCII I3 ASCII I3 ASCII Init String SFX4V1E0F1 Dial String Hangup String T+++*~~ATH0 Dialing Timeout 30 seconds	Instrument Size Small Medium Large Full Msg Sep 10 ASCII Terminator Scm Ref every 15 sec Remote Display Enable Data Record Loading Save to file ← Create Append Raw Flags	Ethenet ESC 0832 Enable IP addr Direct TCP/IF rable

- 3) Click "OK"
- 4) Click "Instrument" and go to "TCP Connect" then "IP addresses"
- 5) Enter the IP address of the instrument and click "OK"



6) Go to "Instrument" and "TCP Connect" and click "Connect"

Connect to a 49iQ using ePort (only TCP/IP)

- 1) When running ePort for the first time, chose "create new configuration"
- 2) Click on "Instrument" and then "New Instrument"
- 3) Choose a name for "Instrument Name." Enter the IP address of the 49iQ instrument. Choose a "Group" name. Don't check the "Password" box. The instrument name and Group does not matter, but it is required that something be entered.

ePort			\times
File Instrument Help			
	Add New Instrument Instrument Name 49Q IP Address 192.168.0.49 Group Boulder OK Cancel		
Ready		New Co	onfig 🔡

- 4) Click "OK" It will take a few seconds to set-up.
- 5) Click on "Yes" on the "Start Download Setup Wizard" Box that eventually opens.

Appendix B - Using FileZilla FTP

You may use any ftp program, but if you choose FileZilla:

- 1) Download FileZilla from http://filezilla-project.org/ Choose the "FileZilla Client" option
- 2) Install FileZilla to the desktop of you r computer
- 3) Open FileZilla
- 4) To log into FileZilla through quick connect at the top of the window:
 - a. Host = awftp.cmdl.noaa.gov
 - b. User=anonymous
 - c. Password =[your full email address]
- 5) Directories are invisible for security reasons, so to get to your directory:
 - a. Go to Remote site: address bar, type /data/ozwv/surface/xxx
 - Where xxx is your station three letter code (see table below)
- 6) From the "local" side of the screen (left side) find the files for transfer in the following folder

path: C:\Program Files\Thermo\iPort\

- 7) Transfer both the .lrc and .src files from the "Local" side of the screen to the "Remote" side of the screen by selecting the files and dragging them to the remote directory.
- 8) Close FileZilla

Station	Code
Arrival Heights	ARH
Erie, CO	BAO
Barbados	BAR
Bermuda	BER
Barrow, AK	BRW
Lauder, New Zealand	LDR
Mauna Loa, HI	MLO
Niwot Ridge, CO	NWR
Pico, Portugal	PCO

Station	Code
American Samoa	SMO
South Pole	SPO
Summit, Greenland	SUM
Trinidad Head, CA	TDH
Tiksi, Russia	ТІК
Tundra Lab, CO	TUN
Moody, TX	WKT
Weaverville, CA	WVR

Appendix C – Pump Replacement / Rebuilds.

Note, some years ago, the manufacturer of the internal pumps for Thermo Fisher Scientific 49C and 49i ozone analyzers stopped manufacturing that type of pump. The newer pumps come from a different manufacturer. The two are slightly different. See the pictures below for the difference.

For pump replacement/rebuild instructions please see the below links. Contact Peter Effertz if you are unsure of the exact methods.

49C/I 'Old Style'	49C manual
49C/I 'new style'	https://assets.thermofisher.com/TFS-Assets/EPM/Part-Lists/EPM-
	iSeriesPumpsTB11111P1.pdf
49iQ	49iQ manual

However, below are some pictures for quick reference.

Pump diagram for the 'old' style 49C/I pumps.



Pump diagram for "new" style 49C/I pumps:





49iQ internal pump





Figure 5–2. Pump Rebuilding

Replacing 49C/I pump





Figure 5-1. Capillary Location

Replacing 49iQ pump



Appendix D – Changing External Savillex Filter

There are two types of filters that are used with the TEI 49 ozone analyzers:

Inline filter is shown to the left. The bell filter is placed on the end of the sample inlet and is open to the atmosphere. In both filters, the orange plastic port is filtered air, the clear is the input air (see the arrow on the clear part.

- 1) Unscrew filter assembly using the wrenches
- 2) Remove old filter
- 3) Replace with new filter and re-assemble. Use the wrench to tighten just past "Hand tight"



Appendix E – Cleaning Capillaries

When the flow readings are different in the two cells of the TEI, or if both flows are near zero with the pump running, the problem may be a blocked capillary.

- 1) Open the lid of the TEI. You should see the internal pump. An inlet and outlet are located on top of this pump. The inlet has a T-connector with two tubes coming in.
- 2) Loosen the nuts on the INLET allowing the tubing and glass capillary to be removed from each nut.
- 3) The glass capillary may be clogged, so take something very thin to push out debris. A multi-strand wire (less than 0.015" diameter wire). Unwind it, using one strand of wire, pushing it through the tiny hole that goes through the capillary.
- 4) Do this for both glass capillaries.
- 5) Replace capillaries and tighten nuts.
- 6) Check instrument flow in both cells.