Trace Organic Gas Analyzer (TOGA)

Operation Manual

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The Trace Organic Gas Analyzer (TOGA) has been developed to measure trace organic compounds on the Hiaper G-V platform from low altitude to 50 kft, sampling at all temperatures and in all weather conditions. 40 selected organic species are measured at all atmospheric concentrations with detection limits variable but extending to the part per quadrillion (ppqv) level.

Contact Eric Apel or Alan Hills for any issues regarding TOGA operation (contact information is on the cover of this Operation Manual).

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A. Theory of Operation

The Trace Organic Gas Analyzer (TOGA) was based on over 10 years of precursor Fast Gas Chromatograph Mass Spectrometer (FGCMS) instruments which were flown worldwide on propeller and jet aircraft in many scientific campaigns. Continuous development of the FGCMS instruments refined the technique and ultimately resulted in the single-rack TOGA instrument.

The instrument is modular and individual components can be serviced, upgraded and even replaced over time so that TOGA can continue to improve. At present the instrument measures 40 selected organic species with 40 second time resolution on a 2:00 minute repeating cycle for the duration of a HIAPER flight. After a pre-flight setup TOGA runs unattended for a 14 hour time block (and then needs an LN_2 recharge). An in-instrument calibration system produces zero air and calibration mixtures for each of the 40 selected measurement species. The compounds measured are flexible and can be nearly any organic species in the C2-C10 molecular structure range and can consist of alkanes, alkenes, alkynes, chlorofluorocarbons, halons, and reactive oxygenated species (such as alcohols, ketones, esters, acids). Such a diverse and selectable compound measurement suite, over such a broad measurement range, has not been accessible with an in-situ instrument prior to TOGA.

Sample handling/analysis

TOGA's air sample handling schematic is shown below. Air (at ~2 slpm) is sampled via a temperature controlled Himmel inlet. After the Himmel inlet the air is routed through electropolished stainless tubing, first to a mass flow controller, then to a stainless bellows pump and then vented out of the aircraft. For 40 seconds out of each 2 minute cycle, a small aliquot of the main 2 slpm flow (~45 sccm) is routed through an elaborate preconcentration system where the air is first dried, the trace organic constituents are enriched by discriminating against N2 and O2, cryofocused and are then separated via a custom gas chromatograph and finally quantified in a modified Agilent (5973) mass spectrometer. The time resolution of the measurement is that due to sampling (40 seconds). Pre-concentration and analysis are tuned to exactly 2:00 minutes each, so even though time resolution is 40 seconds, the end of the analysis is shifted in time 4:00 minutes from the instant sampling occurred.

The complex sample handling/analysis is automated via LabVIEW software written for TOGA/HIAPER. A screenshot of the software is shown in Figure 2.

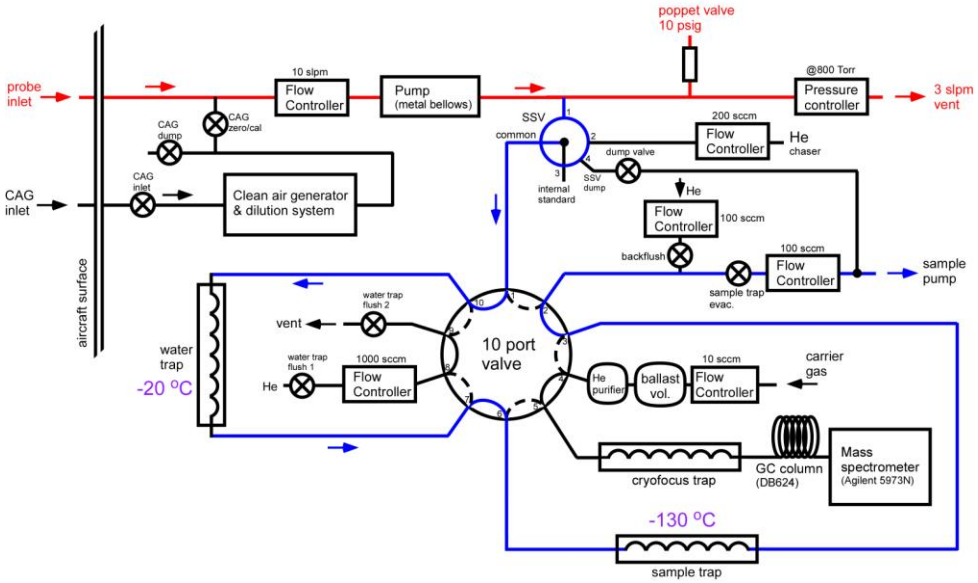


Figure 1. TOGA sample preconcentration/analysis flow schematic.

Figure 2. TOGA LabVIEW software graphical user interface (GUI).

B. TOGA components

The instrument consists of six major components which are housed in a single Hiaper rack. They are:

1. Pump box
2. Clean air generator/calibrator
3. Electronics box
4. MS electronics/Flow controllers
5. MS chamber and high vacuum pumps
6. LN_2 dewar assembly

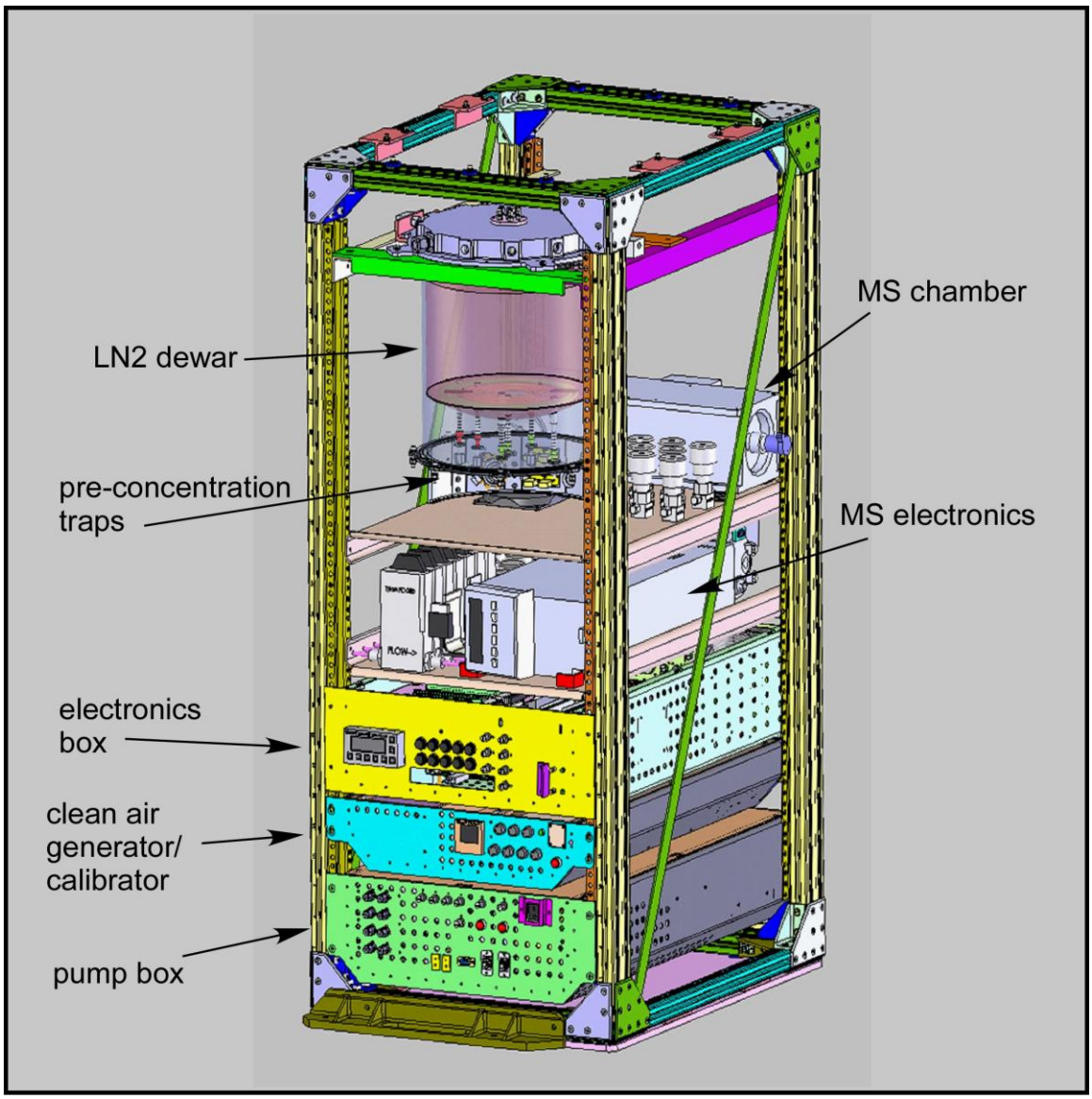
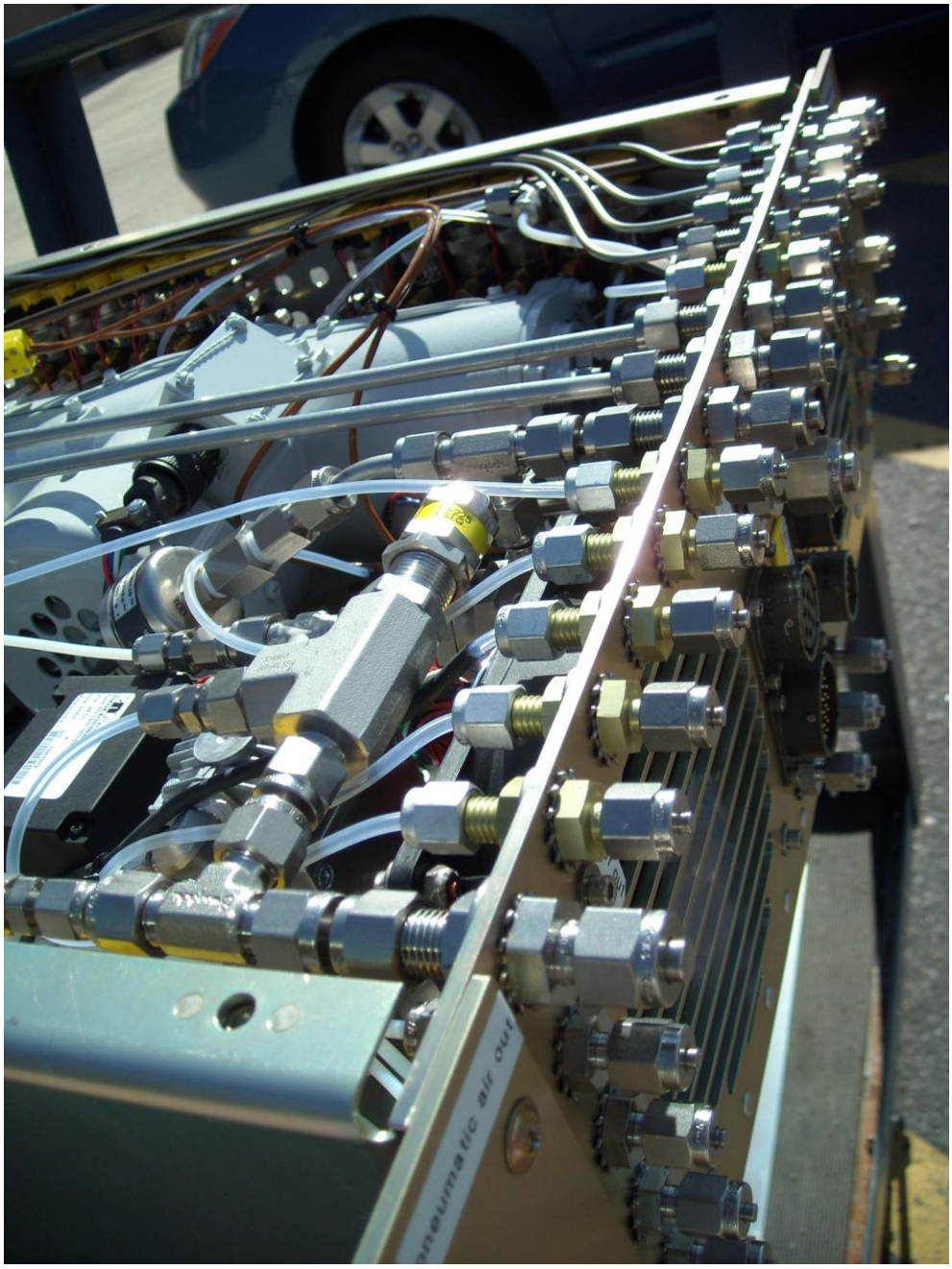


Figure 3. TOGA rack-mounted components.

1. Pump box

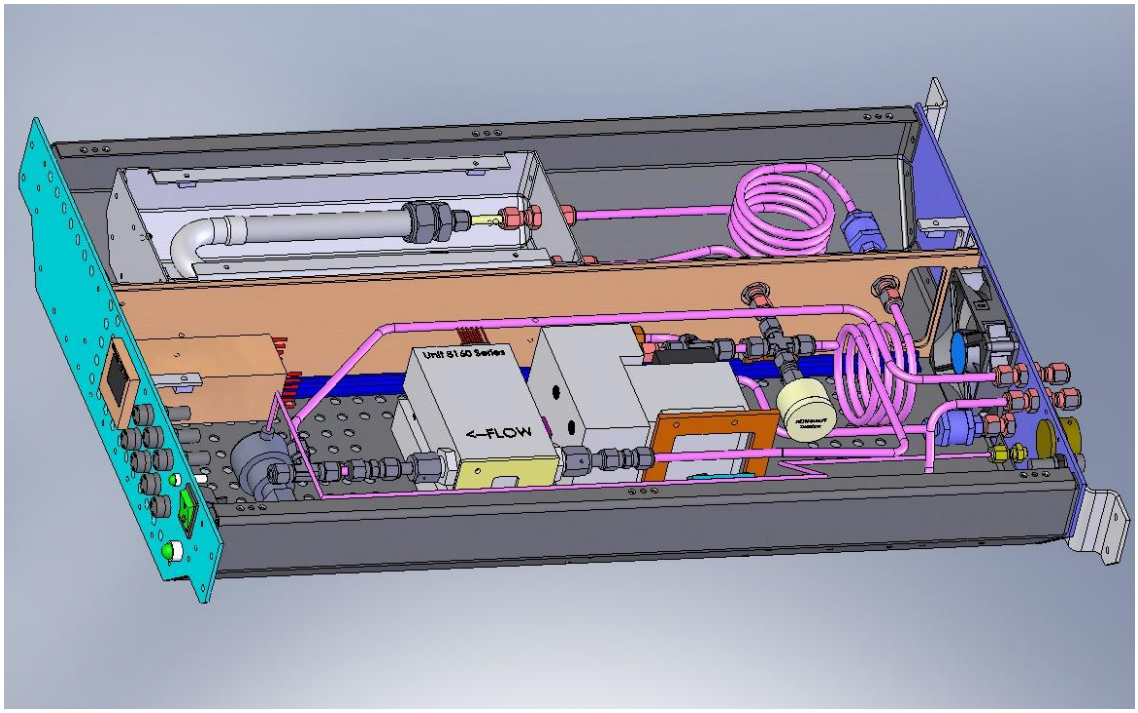
The pump box houses 1.) the main bellows pump to pull air from outside the aircraft into the instrument, 2.) a pneumatic pump to generate pressure to drive the pneumatically actuated valves, and 3.) a roughing pump which pulls sample air through the traps and provides a rough vacuum for the MS system.



The large number of ports on the rear of pump box provide connections to the pneumatic valves TOGA uses primarily for sample preconcentration.

Pump box continued – rear top view.

2. Clean air generator/calibrator (CAG)



The clean air generator/calibrator (CAG) pulls in ambient air at 3 slpm and pushes the air through a heated platinum catalyst. This oxidizes all organic compounds in the air (to <0.010 pptv), providing an ultra-clean air source for zeroing the instrument. The CAG also has the capability of mixing a cylinder standard into the purified air providing calibration mixtures to TOGA at concentrations of 0 to ppb level for the chosen 40 organic components. The CAG is remarkable in that the zero air generated is cleaner than any cylinder air available for purchase and it preserves the measurement air matrix which could affect instrument zero/calibration.

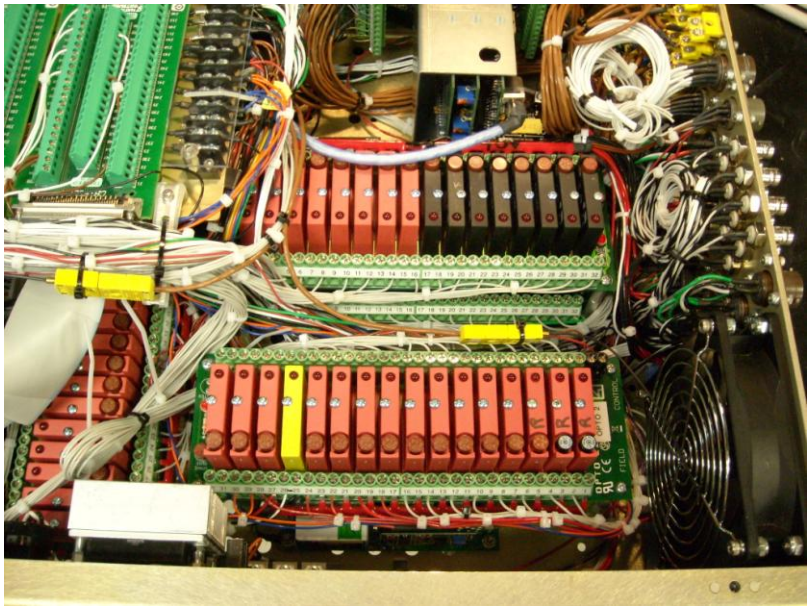
3. Electronics box

The electronic box houses the computer system, a 32 channel Watlow temperature controller and thermocouple measurement interface, 70 channels of OPTO power module switching, DC/DC conversion and the molecular drag pump electronics.

The computer is an Intel DG43NB ATX board with a 500 GB SATA drive, 4096 MB of PC6400 DDR2 RAM with a Core 2 Duo E8400 3GHz CPU. Four data acquisition boards provide DAQ to TOGA they are National Instruments:

- PCIe-6343; 32 analog in, 4 analog out and 48 digital I/O lines
- PCI-6259; 32 analog in, 4 analog out and 48 digital I/O lines
- PCI-6713, 8 channel analog out
- PCI-8430/4, 4 channel serial

LabVIEW based software controls all aspects of TOGA operation including power up and power down.



TOGA Electronics box. Thermocouple breakout connectors and OPTO power modules are pictured.

4. Mass spectrometer electronics/Flow controllers

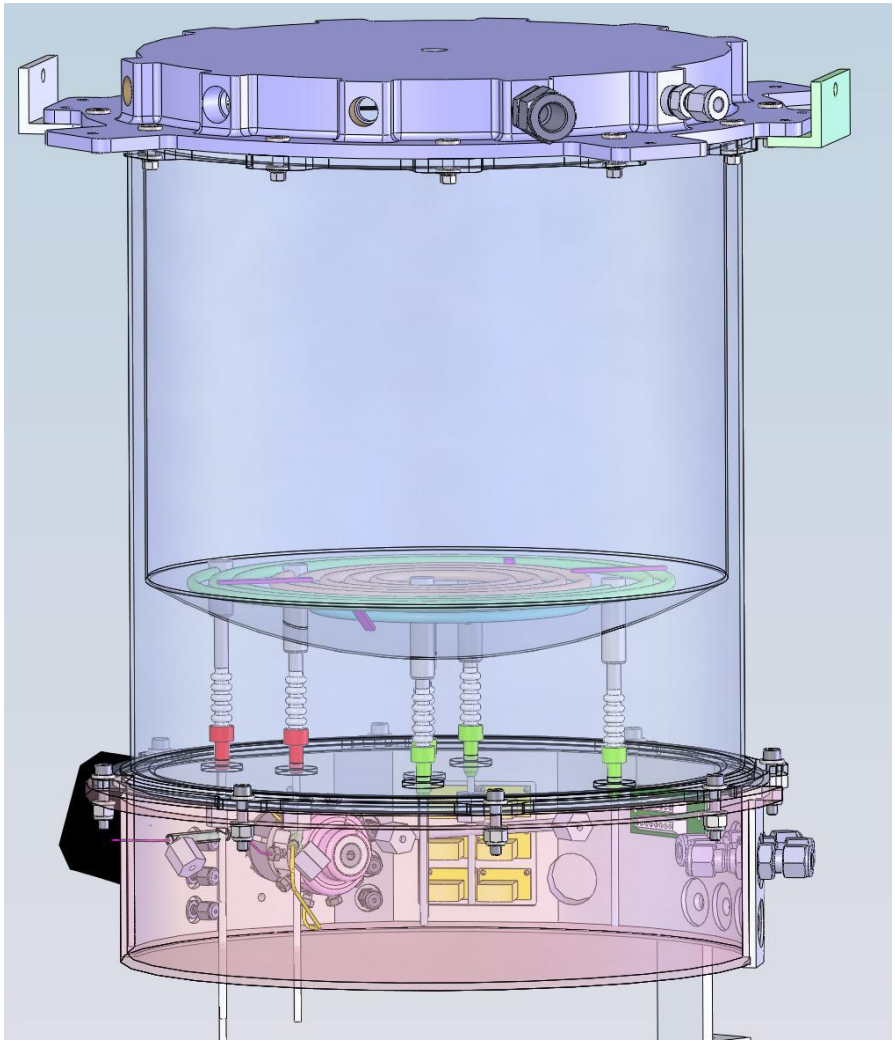
On a shelf at mid-height in TOGA reside twelve mass flow controllers, the MS electronics module, and the pneumatic valves.

5. Mass spectrometer chamber and high vacuum pumps

Above and just behind the flow controller shelf is the MS chamber, gas chromatograph, as well as the turbomolecular and molecular drag pumps. These pumps provide the first and second stage pumping for the MS analysis chamber.

6. LN_2 dewar assembly

The uppermost component in the rack is the liquid nitrogen dewar. The upper part of the dewar contains the reservoir for LN_2. The lower region contains passthroughs for the cooled N2 gas, a 10-port gas valve, and adjacent water/sample/cryofocus traps.



This photo shows the LN_2 heat exchange coils at the base of the dewar, this is where N_2 gas is cooled prior to flow into the organic removal traps.

C. Instrument Setup

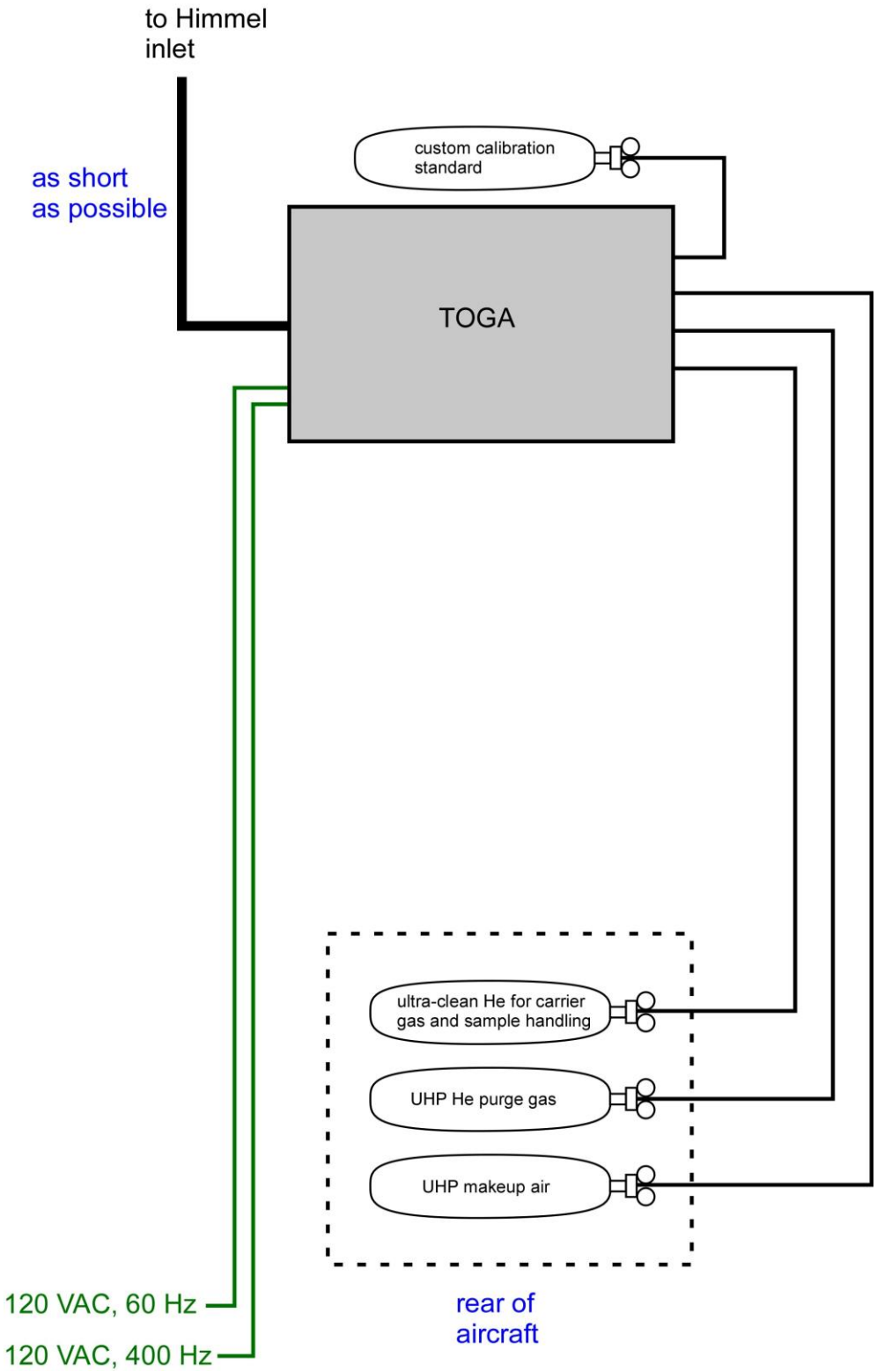
Installation

1. A representative from the Apel group should be on hand to assist in the installation of TOGA onto HIAPER.
2. Mount the special TOGA-modified Himmel inlet at the top of the G-5 cabin.
3. Wheel the TOGA instrument into the correct location.
4. Have the Apel group remove the protective panels on the sides of TOGA.
5. Remove the wheel assemblies on the fore and aft sides of TOGA. Have the Apel group carefully store these specially modified wheel assemblies.
6. Bolt the instrument in place so that the fore side of TOGA is as close as possible to the Himmel inlet.

Connections

Electrical
120 VAC, 60 Hz and 120 VAC, 400 Hz power is used and connects to the bottom box in the rack, the pump box.

Gas connections
Gas lines will be run by the Apel group to the Himmel inlet and to three gas cylinders in the rear of the aircraft. The cylinders are for: 1. Special purity helium for the gas chromatograph, 2. UHP He for purging operations, and 3. UHP air used as makeup air in the clean air generator. A fourth (small) cylinder is used directly in front of the instrument (resting on the floor) for in-flight CAG calibrations.


to Himmel
inlet
as short
as possible
custom calibration
standard
TOGA
ultra-clean He for carrier
gas and sample handling
UHP He purge gas
UHP makeup air
rear of
aircraft
120 VAC, 60 Hz
120 VAC, 400 Hz

D. TOGA Power-up sequence

Pump box (lowest in rack)

1. Request 120 VAC/60 Hz and 120 VAC/400 Hz power from HIAPER personnel
2. Turn on **AC in** (by pushing in the breaker switch)
3. Turn on **UPS**
4. Turn on 2nd **UPS**
5. Turn on **Main power** rocker switch
6. Power up the UPS board by pushing and holding the small black switch below the red/yellow/green LEDs (far right of pump box). The green LED will remain on. If periodic beeping occurs, the aircraft 120 VAC/60 Hz power is not making it to TOGA.
7. Turn on **24 VDC**
8. Turn on **UPS AC out**

Electronics box (third in rack)

9. Turn on **PC pwr** breaker
10. Push up and hold the **PC** toggle switch to begin the PC boot
11. After the PC boots double click on the TOGA LabVIEW software
12. Click on the black arrow (upper right of screen) to start the code running
13. Turn on **AC outlets**
14. Turn on **OPTO 3&4 AC**
15. Turn on **24 VDC outlets**
16. Turn on **24 VDC optos**
17. Turn on **24 VDC pumps**

Cylinder check

18. Go to the rear of the aircraft and check the cylinder pressures for: He carrier, He purge and Air makeup. The cylinders should have at least 1000 psig and regulator pressures should be (nominally): 60 psig (He carrier), 30 psig (He purge) and 30 psig (Air makeup). Report low cylinder pressures and incorrect regulator pressures to the Apel group. **These must be correct prior to flight.**

Dewar system

19. Open dewar **vent** valve to release any residual pressure. Confirm pressure is close to zero by viewing dewar pressure readout on main screen.
20. Open LN2 **liquid fill** and LN2 **liquid drain** valves
21. Carefully add ~10 L of LN2 to dewar. Top off dewar as needed to fill the dewar. **DO NOT OVERFILL THE DEWAR!** That will damage the dewar system.

22. Close the LN2 **liquid fill** and LN2 **liquid drain** valves
23. Close the dewar **vent valve**
24. Build N2 dewar pressure to 11 psig by clicking on the **LN2 dewar heat** switch (on the main program graphical user interface, GUI). Observe that N2 pressure builds up to ~11 psig during the dewar heat cycle

Start TOGA measurement mode

25. Observe that the system is operating normally after power-up.
    - all pumps are working
    - rough pressure is <10 Torr
    - ion gauge pressure is $<10^{-5}$ Torr
    - He carrier is ~1 sccm
    - N2 dewar pressure is ~11 psig

26. Engage TOGA measurement by changing mode from **standby** to **measurement.** The instrument is now performing it's cyclic operation but is not yet sampling outside air.

1 hour prior to takeoff

27. Have ground crew remove Himmel probe cover.

At takeoff

28. Change inlet control from **standby** to **sample**. TOGA is now sampling outside air and performing trace organic gas measurements.

In-flight calibration

29. Perform instrument zero and calibrations using the software, as instructed by the Apel group and on the schedule agreed to pre-flight

Prior to touchdown

30. Change inlet control from **sample** to **standby**.

E. TOGA shutdown

1. Click on the automated instrument **shutdown** function and carefully monitor the shutdown procedure as the software executes the many step procedure. **DO NOT ALLOW AIRCRAFT POWER TO BE PULLED PRIOR TO COMPLETION OF THE SHUTDOWN PROCEDURE!!!** Doing so would damage TOGA severely!

The shutdown algorithm, counts down, prominently displays "**time until shutdown**" so the remaining shutdown time can be accurately relayed to Hiaper personnel as needed. Total shutdown requires 8 minutes.

2. When the automated shutdown is complete the code will popup: "Automated TOGA shutdown complete", close LabVIEW and using the Windows Start function, have Windows turn off the computer.

3. Also turn off the MS computer from Windows.

After landing

4. Have ground crew reinstall Himmel probe cover

F. Operating parameters

Parameter	Instrument specific value
Regulator pressure for ultra-clean He carrier/sample handling gas	60 psig
UHP He, purge gas	30 psig
UHP air, makeup gas	30 psig
Custom calibration standard	30 psig
LN2 pressure (nominal after LabVIEW pressure build cycle)	11 psig
Carrier gas flow rate	1 sccm
Purge gas flow rate	0 sccm in flight 20 sccm ALL other times (critical orifice controlled)
Makeup gas	0-2 slpm variable as required during flight calibrations
Himmel -> TOGA primary sample air flow	2 slpm
TOGA preconcentration air flow	45 sccm, intermittent

G. TOGA Calibration

Calibrations are automatic based on pre-set or set in-flight values. Typically TOGA will run calibrations once/hour regardless of aircraft speed/altitude etc. An on-board operator can turn the periodic calibrations off or cancel an upcoming calibration by clicking on a button on the control screen.

H. Precautions

- Wear safety glasses and gloves during LN_2 fill operations
- Do not overfill the LN_2 dewar. Fill level can be monitored in real-time on via the LabVIEW GUI
- **Do not cut power to TOGA without it first executing its normal power down procedure.** If power needs to be cut push the "powerdown" button and wait for it to shut down automatically. It will sequence through various procedures and then shut off the PC. When the PC shuts off power to TOGA may be cut. The shutdown sequence time is 8 minutes. During the shutdown sequence, the remaining time will be prominently displayed on screen. Cutting power to TOGA without letting it execute a normal shutdown can damage the mass spectrometer and turbomolecular pump.
- **Do not engage TOGA sample mode unless in flight.** Engaging sample modes at other times can irreversibly contaminate the instrument which is ultrasensitive to the chemicals present on the ground at airports and aircraft hangars.
- Keep TOGA Himmel probe cover in place at all times during ground operations and during down days.