Air Quality: Flights, Theory, and Data



Dr. David Delene University of North Dakota

Air Quality Health Effects

Each 10 ug/m³ elevation in fine particulate air pollution was associated with:

4 % increased all cause morality6% increased cardiopulmonary mortality8% increased risk lung cancer mortality



Image by Fred Remer June 30, 2015 over North Dakota

Exposure-Response Curve



The curve is based on a natural spline with 2 df estimated from the residual relative risk of death within a metropolitan statistical area (MSA) according to a randomeffects survival model. The dashed lines indicate the 95% confidence interval of fit, and the hash marks indicate the ozone levels of each of the 96 MSAs. Ref: Jerrett M et al. N Engl J Med 2009;360:1085-1095

CH423 Air Quality Measurements





U.S. SO₂ Emission

Main source is coal combustion





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FORMATION OF SULFATE-NITRATE-AMMONIUM AEROSOLS

$$H_2SO_4(g) \xrightarrow{H_2^0} SO_4^{2-} + 2H^+$$
$$NH_3(g) \xrightarrow{H_2^0} NH_4^+ + OH^-$$

$$HNO_3(g) \xrightarrow{H_2^0} NO_3^- + H^+$$

Thermodynamic Rules:

Sulfate always forms an aqueous aerosol

Ammonia dissolves in the sulfate aerosol totally or until titration of acidity, whichever happens first

Nitrate is taken up by aerosol if (and only if) excess NH_3 is available after sulfate titration

$NH_3(g) + HNO_3(g) \rightarrow NH_4NO_3(aeroso)$	<i>l</i>)
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 HNO_3 and excess NH_3 can also form a solid aerosol if RH is low

Condition	aerosol pH	Low RH	High RH
[S(VI)] > 2[N(-III)]	acid	H ₂ SO ₄ •nH ₂ O, NH ₄ HSO ₄ , (NH ₄) ₂ SO ₄	(NH ₄ ⁺ , H ⁺ , SO ₄ ²⁻) solution
$[S(VI)] \leq 2[N(-III)]$	neutral	$(NH_4)_2 SO_4$, NH ₄ NO ₃	(NH_4^+, NO_3^-) solution

Courtesy of Daniel J. Jacob

Flight Forecasting



August 24, 2013 MODIS Terra image showing an impressive thickness of the smoke from the Rim Fire in California but solar viewing angle and the smoke being on the eastern half of the swath may have exaggerated the optical thickness.

<u>MODIS Fire Detection</u> 08/29/2013 - 09/07/2013



Fire maps accumulates the locations of the fires detected by MODIS on board the Terra and Aqua satellites over a 10-day period. Each colored dot indicates a location where MODIS detected at least one fire during the compositing period.

NOAA Fires and Smoke from Satellite Tool



National Weather Service

1 HR Ozone Valid 7 pm SEP 01, 2015



Flight Planning: Air Quality Missions



- Takes time for gas analyzers to warm up.
- Instrument have different time responses.

Ozone and Air Quality



1.278 Å

116.78°

Ozone Measurement Principle of Operations

- Ozone measurement is based on absorption of ultraviolet light (UV) at 254 nm.
- Amount of UV absorption is described by Beer-Lambert Law.

$$\frac{I}{I_0} = e^{(-KLC)}$$

- K = Molecular Absorption Coefficient, 308 cm⁻¹ (at 0 °C and 1 atmosphere)
- L = Length of Cell (38 cm for Model 49C)
- C = Ozone Concentration in parts per million (ppm)
- I = UV Light Intensity of Sample with Ozone (Sample Gas)
- I = UV Light Intensity of Sample without Ozone (Reference Gas)

Photochemical Formation of Ozone From Nitrogen Dioxide

 $NO_2 + hv \rightarrow NO + O$ $\lambda < 430 \text{ nm}$

$$O + O_2 + M \rightarrow O_3 + M$$

$$NO + O_3 \rightarrow NO_2 + O_2$$

What does M represent?

What does λ represent?

Scheme for O_3 by Oxidation of Carbon in Presence of NO_x

 $RH + OH \rightarrow R + H_{2}O$ $R \cdot + O_2 + M \rightarrow RO_2 \cdot + M$ $RO_{2} + NO \rightarrow RO + NO_{2}$ $RO + O_2 \rightarrow HO_2 + R'CHO$ $HO_2 \cdot + NO \rightarrow OH \cdot + NO_2$ $2[NO_{2} + hv \rightarrow NO + O]$ $2[O + O_2 + M \rightarrow O_3 + M]$

What does R represent?

What does R' represent?

Net: $RH + 4O_2 + 2hv \rightarrow R'CHO + H_2O + 2O_3$

Oxidation of Methane Mechanism: NMVOC Concentration is Low

 $CH_{A} + OH \rightarrow CH_{3} + H_{2}O$ $CH_{2} + O_{2} + M \rightarrow CH_{2}O_{2} + M$ $CH_{3}O_{2} + NO \rightarrow CH_{3}O + NO_{2}$ $CH_{2}O + O_{2} \rightarrow HO_{2} + CH_{2}O$ $HO_2 \cdot + NO \rightarrow OH \cdot + NO_2$ $2[NO_{2} + hv \rightarrow NO + O]$ $2[O + O_2 + M \rightarrow O_3 + M]$

What does NMVOC represent?

Net: $CH_4 + 4O_2 + 2hv \rightarrow CH_2O + H_2O + 2O_3$

Carbon Monoxide Mechanism:

 $CO + OH \rightarrow CO_{2} + H \rightarrow HO_{2} + M$ $H \rightarrow O_{2} + M \rightarrow HO_{2} + M$ $HO_{2} + NO \rightarrow OH + NO_{2}$ $NO_{2} + hv \rightarrow NO + O$ $O + O_{2} + M \rightarrow O_{3} + M$

Net: $CO + 2O_2 + hv \rightarrow CO_2 + O_3$

Remove of Ozone Deposition onto Earth's Surface

Photochemical Lost:

$$O_{3} + hv \rightarrow O_{2} + O_{2}$$
$$O_{2} + H_{2}O \rightarrow 2OH$$
$$HO_{2} + O_{3} \rightarrow OH + 2O_{2}$$

Lifetime of Ozone in Troposphere Season | Altitude | 40 °N Lat | 20 °N Lat

Summer|0 km |8 days | 5 days Winter|0 km |100 days| 17 days

Summer|5 km | 15 days| 10 days Winter|5 km |160 days| 35 days

Summer|10 km | 40 days| 30 days Winter|10 km |300 days| 90 days

Ambient Ozone Trend



Ref: Air Pollution: Engineering, Science, and Policy by Steven Sternberg, Figure 12-4

Ozone Isopleths



Ref: Air Pollution: Engineering, Science, and Policy by Steven Sternberg, Figure 12-5

Thermo Electron Corporation Model 49C Flow Schematic



Pump

Thermo Electron Corporation Model 49C Specifications

- Range 0 0.05 to 1.0 ppm
- Averaging Time 10 to 300 seconds
- Temperature Range 20 to 30 °C
- Line Voltage
 - 90 to 110 VAC @ 50/60 Hertz
 - 105 to 125 VAC @ 50/60 Hertz
 - 210 to 250 VAC @ 50/60 Hertz
- Pressure Compensation on or off
- Temperature Compensation on or off
- Flow Rate 1 to 3 LPM

Ozone Calibration Setup Zero Air – Has < 0.1 ppm of Hydrocarbons



Thermo Fisher Scientific 49i UV Photometric O₃ Gas Analyzer (O3)



- **Operating Principles** Photometric **Primary Measurements** – Concentration of O₃
- **Quality Control** Calibration with Gas Standard **Flight Profile Consideration**
- Long Legs to Average,
 Rapid Pressure Changes
 Data Acquisition
- Serial Data

Time series plot of O_{3} concentration taken during the 13 March 2017 flight near Fargo, North Dakota.



Thermo Fisher Scientific 43i TLE SO₂ Pulsed Fluorescence Gas Analyzer (SO2)

- **Operating Principles** Pulsed Fluorescence **Primary Measurements** – Concentration of SO₂
- Quality Control Calibration with Gas Standard Flight Profile Consideration

Long Legs to Average,
Rapid Pressure Changes
Data Acquisition
Serial Data

Time series plot of SO_2 concentration taken during the 8 March 2017 flight near Fargo, North Dakota.



Thermo Fisher Scientific 42i TL NOx Chemiluminescent Gas Analyzer Operating Principles – Chemiluminescence **Primary Measurements** – Concentration of NO, NO_{γ} , and NO_{x} **Quality Control** – Calibration with Zero Air (Stand Along Generator) **Flight Profile Consideration** 15.78 VOX_Conc [ppb – Long Legs to Average, 10.24 Rapid Pressure Changes, 4.69 Long Heat Up Times **Data Acquisition** – -0.85 └─ 7.80× 7.98×10^{4} 8.04×10^4 Time [sfm] Time series plot of NOx concentration taken during Serial Data the 13 March 2017 flight near Fargo, North Dakota.

Thermo Fisher Scientific 42i-Y NO Chemiluminescent Gas Analyzer (NOy) Operating Principles – Chemiluminescence, NOy Converted to NO using Molybdenum Heated **Primary Measurements** – Concentration of NO Quality Control – Calibration with Gas Standard **Flight Profile Consideration** Time [UTC] -0.44 22:10:11 – Long Legs to Average, 21:50:33

Rapid Pressure Changes **Data Acquisition**– Serial Data, 2 A/D

Time series plot of NOy concentration taken during the 13 March 2017 flight near Fargo, North Dakota.



Picarro Cavity Ringdown Spectroscopy (CRDS)



Operating Principles – Cavity Decay Time **Primary Measurements** – Concentration of CO₂

 $CO CH_{A} H_{2}O$ **Quality Control** – **Calibration for Drifts Profile Consideration** – Long Legs to Average **Data Acquisition** – Serial Data



TSI DIFFUSION DRYER 3062- NC

- Desiccant surrounding the aerosol flow path removes excess moisture by diffusional capture.
- The aerosol never comes in contact with the desiccant material si there is minimal particle loss.
- Desiccant regeneration by removal from the Diffusion Dryer and baking it at 120°C.

Cavity Ringdown Spectroscopy (CRDS) Analyzer for Flight Model G2401-m $(CO + CO_{2} + CH_{4} + H_{2}O)$

Performance Specifications	CO ₂ Specification	CH₄ Specification	CO Specification	H₂O Specification
Precision (1-σ over 30 secs, vibration @ 20 Hz, 1g): Guaranteed over below range & operating conditions	≤ 200 ppb	≤ 2 ppb	≤ 30 ppb	≤ 150 ppm
Drift at STP (over 24 hrs) (Peak to peak 50 min average: Guaranteed over below range & operating conditions)	≤ 200 ppb	≤ 1.5 ppb	≤ 15 ppb	≤ 100 ppm <u>+</u> 5% of reading
Drift with Changing Temp (Peak to peak 30 sec average over 3 hrs; 15°C/hr for below operating conditions):	≤ 7.5 ppbv/°C	≤ 0.05 ppbv/°C	≤ 1.5 ppb/°C	N/A
Drift with Changing Pressure (Peak to peak 30 sec average; < 1.4 Torr/sec for below operating conditions):	≤ 700 ppb	≤ 7.5 ppb	≤ 50 ppb	N/A
Operating Range	0 - 1000 ppm	0 - 20 ppm	0 - 5 ppm	0 – 7 %v H ₂ O / 39 °C dew pt (non-condensing)
Guaranteed Specifications Range	300 – 500 ppm	1 ppm – 3 ppm	0 – 1 ppm	0 – 3 %v H ₂ O / 25 °C dew pt (non-condensing)
Measurement Interval	≤ 3.5 seconds	≤ 3.5 seconds	≤ 3.5 seconds	≤ 3.5 seconds
Rise/Fall time (10-90%/90-10%)	≤ 3 seconds	≤ 3 seconds	≤ 3 seconds	N/A

Atmospheric Concentrations 400 ppm

1875 ppb 100 ppb

CRDS Calibration





Aventech Aircraft Integrated Meteorological Measurement System Probe (AIMMS)



Operating Principles – Gust Probe and IMU coupled to a Differential GPS **Primary Measurements** – Velocity Relative to Air/Ground (Atmospheric Winds) **Quality Control** – Special Flight Profiles **Flight Profile Consideration** – Air Flow **Changes Require Calibration Data Acquisition** – 1.0 H Serial Data

Measuring Wind Via Aircraft

• The wind is given by $V = V_a + V_p$

where V_a is the aircraft velocity relative to the air (true airspeed or TAS) and V_p is the aircraft velocity relative to the ground (ground speed or GS).

• The equation above assumes that the measurement locations of TAS and GS are the same. When they are not, rotation of the aircraft can cause winds at the probe that are not real. Taking this effect into account, the full wind equation is

where Ω is the 3-D angular rotation of the aircraft and R is the position of the probe relative to the INS (Lenschow 1986).

Aircraft and Instrumentation

An Aircraft Integrated Meteorological Measurement System (AIMMS) made by Aventech has been deployed on a many King Air research aircraft

AIMMS Components

- 1. Air Data Probe
- 2. Differential GPS
- 3. Inertial measurement unit (IMU)
- 4. Central processing module (CPM)



Gust Probe

- The gust probe includes pressure transducers to measure vertical, horizontal, and pitot-static differential pressure.
- Temperature and relative humidity sensors are also included in the probe.



Flight Maneuvers





While pressure transducers used to measure pressures on an aircraft can be calibrated on the ground, flow deceleration and deflection around the wing can result in airflow angles and slower airflow speeds (Macpherson and Baumgardner 1988) causing incorrect dynamic pressure and static pressure measurements at the probe's center port.

AIMMS Calibration Model Equations

 Angle of attack (α), angle of sideslip (β), and static pressure error (C_p) are modeled by the following equations:

$$\alpha = a_0 + \left(\frac{P_U - P_L}{P_d - P_s}\right)a_\alpha + \left(\frac{P_r - P_l}{P_d - P_s}\right)a_\beta$$
$$\beta = b + \left(\frac{P_U - P_L}{P_d - P_s}\right)b_\alpha + \left(\frac{P_r - P_l}{P_d - P_s}\right)b_\beta$$
$$C_p = c_0 + \left(\frac{P_U - P_L}{P_d - P_s}\right)c_\alpha + \left(\frac{P_r - P_l}{P_d - P_s}\right)c_\beta$$

where P_U , P_L , P_r , P_l , P_d , and P_s are the upper port pressure, lower port pressure, right port pressure, left port pressure, dynamic pressure, and static pressure. All other variables are calibration constants to be determined. $P_{-}P_{-}$

- C_p is the pressure coefficient at the static ring and is given by where P_{∞} is the true static pressure. $C_p = 1$ at a stagnation point and $C_p = 0$ when the pressure measured is the true static pressure.
- All maneuvers are performed high above the boundary layer so that a uniform, non-turbulent wind field can be assumed.
- Vertical wind is assumed to be zero.

AIMMS Calibration Method

- The calibration constants are determined so that the wind vector has the smallest possible dependence aircraft motion.
- This is done by minimizing the difference between mean wind speeds between reverse tracks, assuming zero vertical wind, and minimizing the variance of wind.

$$Var_{total} = Var_{atmos} + Var_{aircraft}$$

• Minimizing the variance of wind comes from the assumption that calibration constants other than the correct ones would result in a larger variance than the actual variance of the wind (Khelif 1999).

AIMMS Performance Check

- A validation flight was performed two days after the calibration flight on 23 March 2009.
- Maneuvers performed at both 15000' and 21000' MSL.



UND Cal. Method – Equation Background

• The full wind equation is again given by

 $V = V_a + V_p + \Omega X R$

where V_a is the aircraft velocity relative to the air (TAS), V_p is the aircraft velocity relative to the ground (GS), Ω is the 3-D angular rotation of the aircraft, and R is the position of the probe relative to the INS.

- Full equations are well known (Lenschow 1986, Khelif 1999) but assume airflow measurements are on the longitudinal axis.
- To take into account the position of a probe on the wing, the **Ω**XR term must be re-derived.

UND Cal. Method – Wind Equations $u = u_p - u_a D^{-1}(sin\psi cos\Theta + tan\beta(cos\psi cos\phi + sin\psi sin\Theta sin\phi))$ $+ tana(sin\psi sin\Theta cos\phi - cos\psi sin\phi))$ + $L(\dot{\Theta}(sin\psi cos\Theta sin\phi + sin\psi sin\Theta cos\phi - cos\psi sin^2\Theta sin\phi)$ $-\dot{\phi}cos\psi cos^2\Theta sin\phi - \dot{\psi}(sin\psi cos\phi - cos\psi sin\Theta sin\phi))$ $v = v_v - u_a D^{-1} (cos\psi cos\Theta - tan\beta(sin\psi cos\phi - cos\psi sin\Theta sin\phi)$ $+ tana(cos\psi sin\Theta cos\phi + sin\psi sin\phi))$ + $L(\dot{\Theta}(\cos\psi\cos\Theta\sin\phi + \cos\psi\sin\Theta\cos\phi + \sin\psi\sin^2\Theta\sin\phi)$ $+\dot{\phi}sin\psi cos^2\Theta sin\phi - \dot{\psi}(sin\psi sin\Theta sin\phi + cos\psi cos\phi))$ $w = w_p - u_a D^{-1}(\sin\Theta - \tan\beta\cos\Theta\sin\phi - \tan\alpha\cos\Theta\cos\phi) + L(\dot{\Theta}\sin\Theta\sin\phi)$ $-\dot{\phi}cos\Theta cos\phi$)

UND Cal. Method – Angle of Attack

• Angle of Attack (α) is found by the same relation used by Aventech

$$\alpha = a_0 + \left(\frac{P_U - P_L}{P_d - P_s}\right)a_\alpha + \left(\frac{P_r - P_l}{P_d - P_s}\right)a_\beta$$

• The calibration constants are found assuming w is equal to zero and by minimizing the variance of w during the porpoise maneuvers.



UND Cal. Method – Angle of Sideslip $\beta = b + \left(\frac{P_U - P_L}{P_d - P_s}\right) b_{\alpha} + \left(\frac{P_r - P_l}{P_d - P_s}\right) b_{\beta}$



UND Cal. Method – True Airspeed

- True airspeed is a function of pitot-static differential pressure, static pressure, temperature, and the ratio of specific heats of the air.
- Again, the pitot-static pressure measured by the gust probe must be calibrated for the effects of the aircraft on the airflow at the probe.
- To take this effect into account, a calibrated pitot-static differential pressure (Q_c) is found assuming the linear relationship
- where S and I are sensitivity and offset calibration constants to be determined and Q is the measured pitot-static differential pressure.
- These constants are determined so that the mean wind vector during reverse heading tracks is minimized.

Results – Level Maneuvers



Box-and-whisker plots of vertical wind measurements during straight and level flight at 15000' MSL performed on 23 March 2009. Black and green plots represent the Aventech and UND solutions respectively. Note: Aventech solution used calibration constants determined on 21 March 2009 while the UND solution used calibration constants determined on 23 March 2009. The star indicates the mean value, the horizontal line within the box is the median value, the top and bottom of the box is the 75th and 25th percentile respectively, and the top and bottom of the whiskers are the 95th and 5th percentiles respectively. True airspeeds for each interval are given.

Porpoise Maneuvers 15000'



Box-and-whisker plots of vertical wind measurements during porpoise maneuvers at 15000' MSL performed on 23 March 2009. Black and green plots represent the Aventech and UND solutions respectively. Note: Aventech solution used calibration constants determined on 21 March 2009 while the UND solution used calibration constants determined on 23 March 2009. True airspeeds for each interval are given.

Summary Statistics

Summary statistics for Aventech and UND solutions. Mean and standard deviations were determined using all vertical wind measurements during each maneuver at both 15000' and 21000'. The mean standard deviation was determined by averaging the standard deviation found during each leg.

Method	Maneuver	Mean [m/s]	Stdev [m/s]	Mean Stdev [m/s]
Avontoch	Level	-0.239	0.2782	0.202
Aventech	Porpoise	-0.229	0.348	0.283
UND	Level	0.003	0.298	0.199
	Porpoise	-0.020	0.331	0.295

Main difference between cal. methods

- The main difference between the two calibration methods is how the pitotstatic differential pressure (Q) is calculated.
- UND:

$$Q_c = S * Q + I$$
$$Q = P_d - P_s$$

• Aventech:

$$Q_{c} = P_{d} - P_{s}$$

$$P_{s} = P_{m} + dP$$

$$dP = Q * (c_{0} + \left(\frac{P_{U} - P_{L}}{Q}\right)c_{\alpha} + \left(\frac{P_{r} - P_{l}}{Q}\right)c_{\beta})$$

• UND assumes calibrated pitot-static pressure a linear function of measured pitot-static pressure, while Aventech takes airspeed and airflow angles into account when finding the calibrated pitot-static pressure.

TAS Differences



Why the differences? Dynamic Pressure

- At high airflow angles, the actual stagnation point on a sphere is located away from the designed stagnation point.
- The measured dynamic pressure is then less than the actual dynamic pressure (found at the actual stagnation point).
- Lower dynamic pressure -> lower airspeed
- Since the Aventech equations take the airflow angles into account, the higher airspeeds at high airflow angles are likely more realistic.



Why the differences? Static Pressure



MacPherson and Baumgardner 1988

True airspeeds vary \pm 10 % of the actual true airspeed around PMS cans on the wing of a King Air

Static Pressure Defect









Time series plot of pressure and true air speed measured by the Aircraft Intergrated Meteorlogical Measurement System during the 2 March 2017 flight near Fargo, North Dakota.



Rosemount Total Air Temperature Sensor (Temp)



Operating Principles – Platinum Resistance Temperature Detector (RTD) **Primary Measurements** – Total Temperature (Air Temperature is Derived) **Quality Control** – Calibration at Manufacturer **Flight Profile Consideration** – Icing if Heat Fails

Data Acquisition – 25 H Voltage using A/D Board



Time series plot of air temperature measured by the Total Air Temperature Sensor taken during the 13 March 2017 flight near Fargo, North Dakota.

Edgetech Dew Point Hygrometer (DEW)



Operating Principles – Chilled Mirrow **Primary Measurements** – Dew Point Temperature (Humidity Parameters are Derived) **Quality Control** – Calibration at Manufacturer **Flight Profile Consideration** – Fast descents/ascents Result in Valid Measurements **Data Acquisition** – 25 H Voltage using A/D Board







Time series plot of dew point temperature from the Edgetech sensor during the 13 March 2017 flight near Fargo, North Dakota.