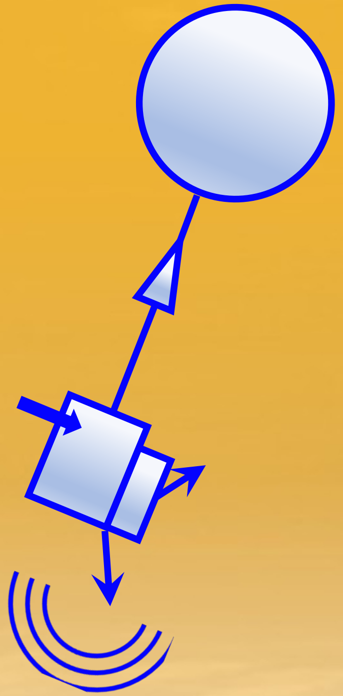
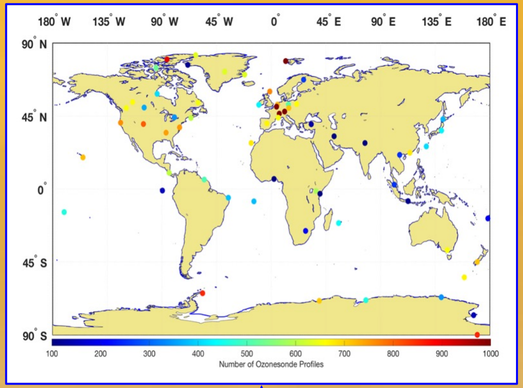
Ozonesonde Measurement Principles and Best Operational Practices

ASOPOS 2.0 (GAW Report No. 268)

(Assessment of Standard Operating Procedures for Ozonesondes)





ASOPOS-Webinar No. 4

Data Processing

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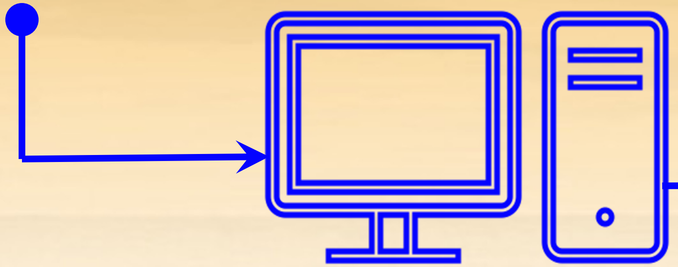
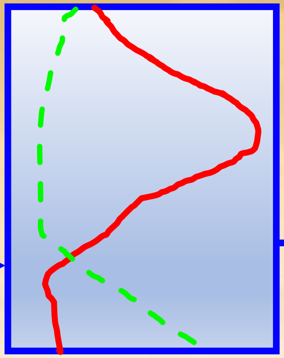
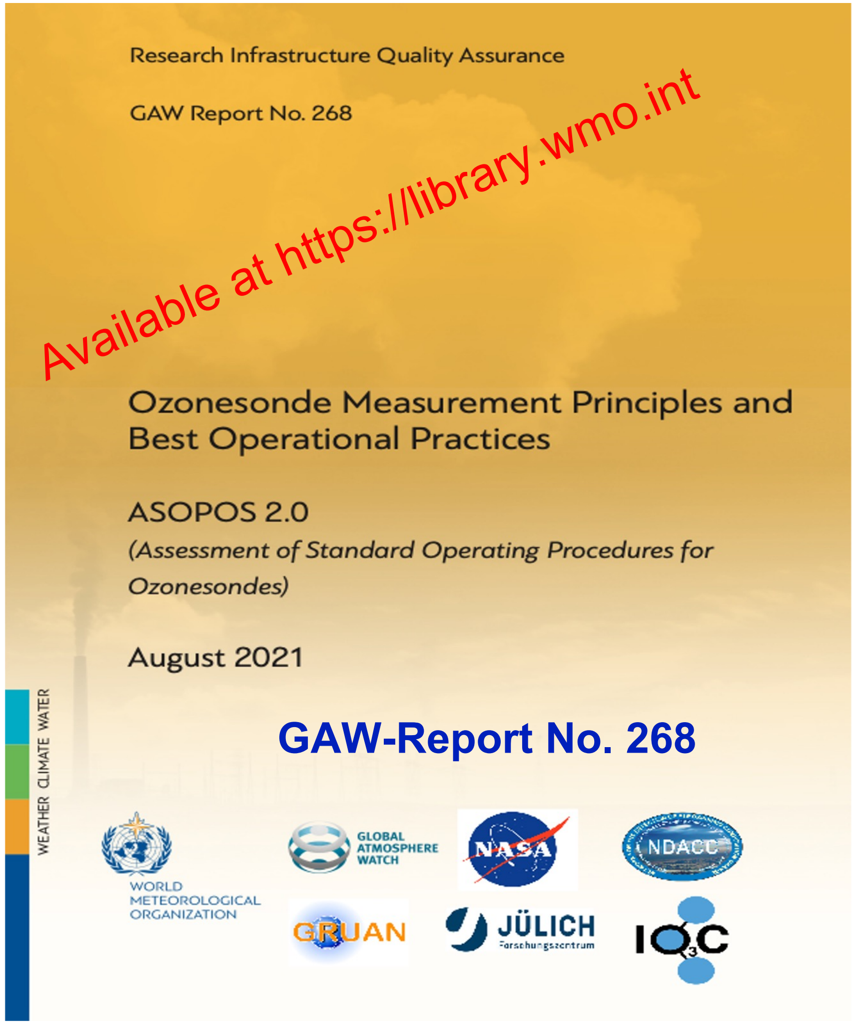




Version March 2024

WORLD METEOROLOGICAL ORGANIZATION · GRUAN · JÜLICH Forschungszentrum · NASA · NDACC · IO3C · GLOBAL ATMOSPHERE WATCH

Preamble


Research Infrastructure Quality Assurance

GAW Report No. 268

Available at https://library.wmo.int

Ozonesonde Measurement Principles and Best Operational Practices

ASOPOS 2.0
(Assessment of Standard Operating Procedures for Ozonesondes)

August 2021

GAW-Report No. 268

WEATHER CLIMATE WATER

WORLD METEOROLOGICAL ORGANIZATION

GLOBAL ATMOSPHERE WATCH

- The focus in this webinar will be not only on the basics of the data processing to derive the ozone partial pressure from the ozonesonde (incl. radiosonde) measurements, but also on new aspects of this ASOPOS 2.0 report, specifically the individual uncertainties of different instrumental parameters that contribute to the overall estimated uncertainty of the ozonesonde data
- The scientific and technical basics of the data processing of ozonesonde data and their uncertainty budget are described in Chapter 3 of the ASOPOS 2.0 Report (WMO/GAW No. 268)
- The ozonesonde data processing in practice is described in detail in Annex-C (WMO/GAW No. 268) : “Practical Guidelines to Determine Ozone Partial Pressure by ECC Sonde, and its associated uncertainty”

Outline

Basic Formula

C_{PH} (E-3-4/E-3-5) "humidification" corr.

C_{PL} (E-3-4) pump temperature corr.

T_M inside pump base
T_P is" truest" pump temperature
$T_M \rightarrow T_P$ (E-3-15)

$\Phi_{PM} = \frac{100}{t_{100}}$
$\Phi_{PM} \rightarrow \Phi_{P0}$ (E-3-3)

$I_B = I_{B1}$ constant

$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P * \eta_A * \eta_C * \Phi_{P0})} * (I_M - I_B)$$

η_P (P) (Table **3-1**):
- SPC + SST1.0/0.5: **K86**
- EN-SCI + SST1.0/0.5: **K95**
- EN-SCI + SST0.1: **NOAA/CMDL 2002 or JMA 2016**

η_A = 1 (3 ml)
$\eta_A \rightarrow$ **E-3-11-A/B** (2.5 ml)

$\eta_C = 1$

- Ozonesonde Parameters
- Flight Time
- Uncertainty Budget
- Individual O_3S-Parameters
- Key Notes

Uncertainty Budget

$\Delta\Phi_{PM}$ = 1% of Φ_{PM}

ΔC_{PH} (E-3-6)

ΔC_{PL} (E-3-8)

ΔI_M = 0.005 µA (I_M < 1 µA)
ΔI_M = 0.5% of I_M (I_M > 1 µA)

ΔI_B = 0.02 µA

ΔT_P = 0.7 K

$\Delta\Phi_{P0}$ (E-3-9)

$$\frac{\Delta P_{O3}}{P_{O3}} = \sqrt{\left(\frac{\Delta\eta_P}{\eta_P}\right)^2 + \left(\frac{\Delta\eta_A}{\eta_A}\right)^2 + \left(\frac{\Delta\eta_C}{\eta_C}\right)^2 + \frac{(\Delta I_M)^2 + (\Delta I_B)^2}{(I_M - I_B)^2} + \left(\frac{\Delta T_P}{T_P}\right)^2 + \left(\frac{\Delta\Phi_{P0}}{\Phi_{P0}}\right)^2 + \sum \varepsilon_i^2}$$

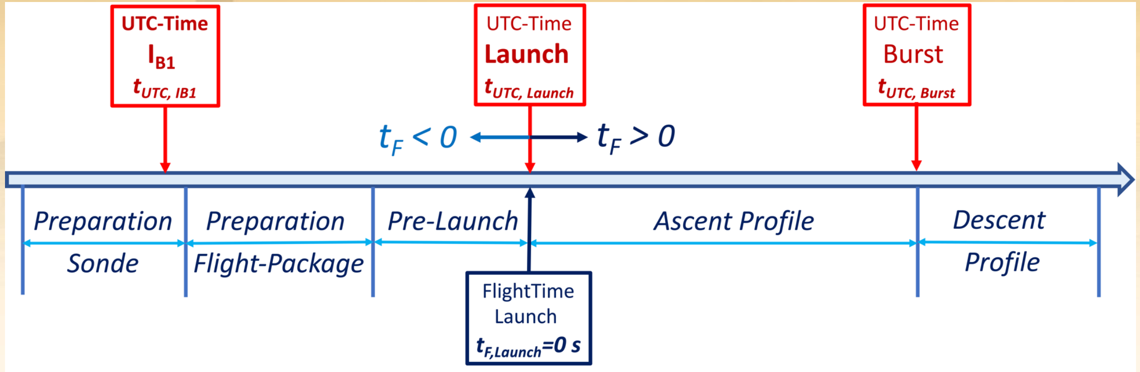
$\Delta\eta_P$ (P) (Table **3-1**):
- SPC + SST1.0/0.5: **K86**
- EN-SCI + SST1.0/0.5: **K95**
- EN-SCI + SST0.1: **NOAA/CMDL 2002 or JMA 2016**

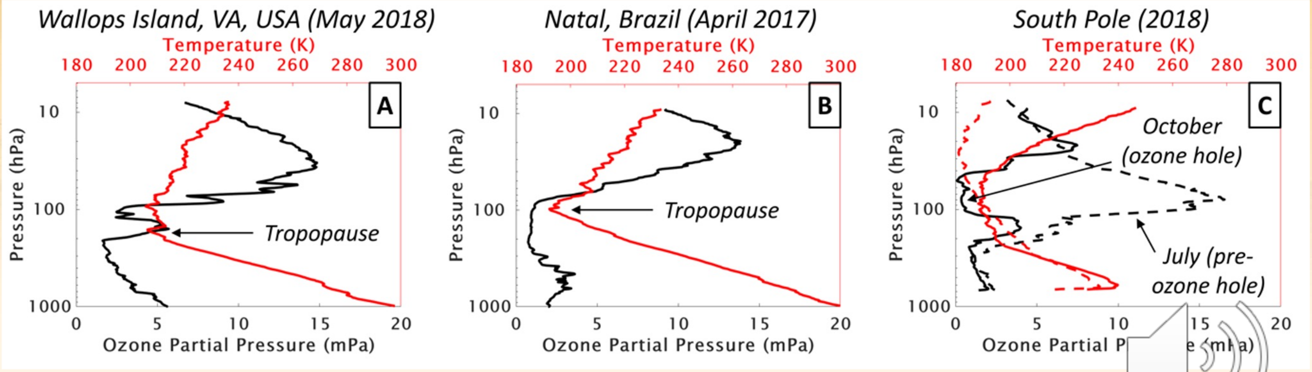
$\Delta\eta_A$ = 0.01 (3 ml)
$\Delta\eta_A \rightarrow$ **E-3-11-C** (2.5 ml)

$\Delta\eta_C$ = 0.03

i=1: ΔF_{trans}
Annex-D: Sect.D-7-10

Flight Time





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Data Processing: Overview *(Section C-3 GAW No.268)*

Basic ECC-Ozonesonde Equation: E-2-1

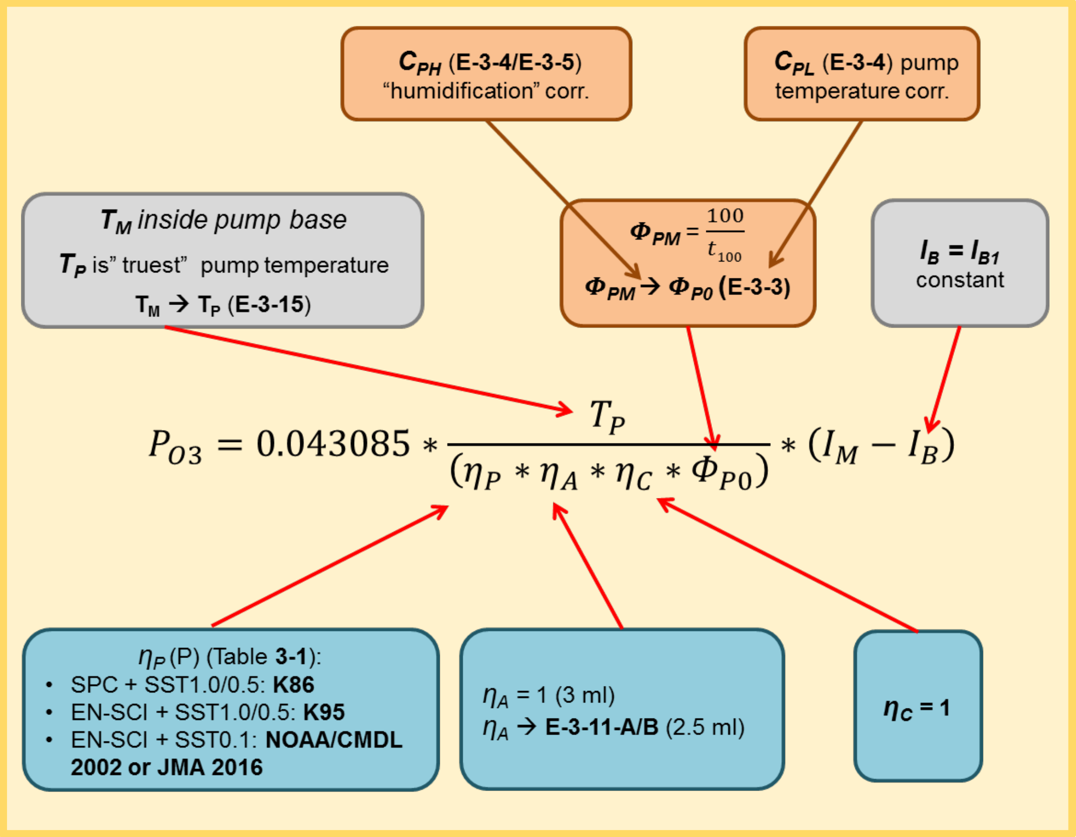


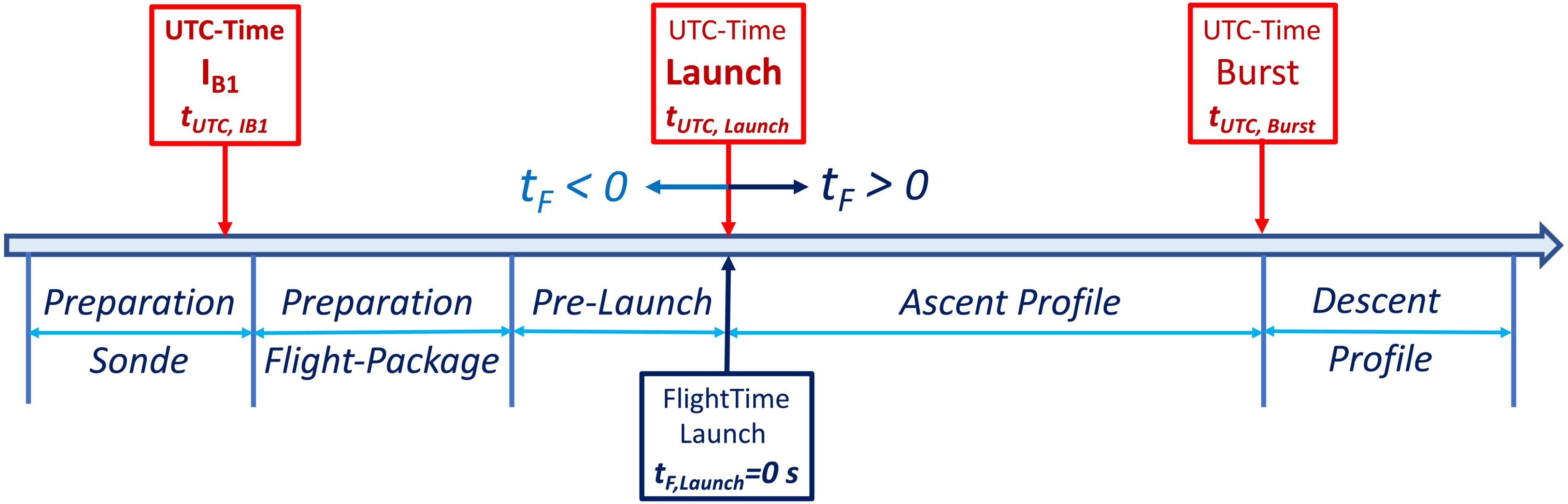
Figure C-3 (Annex-C of WMO/GAW No. 268)

The partial pressure of ozone P_{O3} is derived from the ozonesonde (incl. radiosonde) measurements *(See Left)*:

- **Cell Current** (in-flight): I_M
- **Background Current** (preparation): I_B
- **Pump temperature** (in-flight): from measured T_{PM} to T_P
- **Pump flowrate** at ground (preparation): Φ_{P0}
- **Absorption Efficiency** (empirical): $\eta_A(P)$
- **Pump Efficiency** (empirical): $\eta_P(P)$
- **Conversion Efficiency** (empirical): $\eta_C(P)$
- **Radiosonde** (in-flight):
  - Pressure: P_{Air} ;Temperature: T_{Air} ; Rel. Humidity: U_{Air}
  - GPS: ***Lat, Long, Wind (Velocity & Direction)***
  - Altitude (calculated): ***Z*** or ***H***

⋙ The focus here will be on the most critical parameters and their contributions to the overall uncertainty of the ozonesonde measurement

Flight Time (t_F) as Independent Profile Variable *(Section C-4 GAW No.268)*



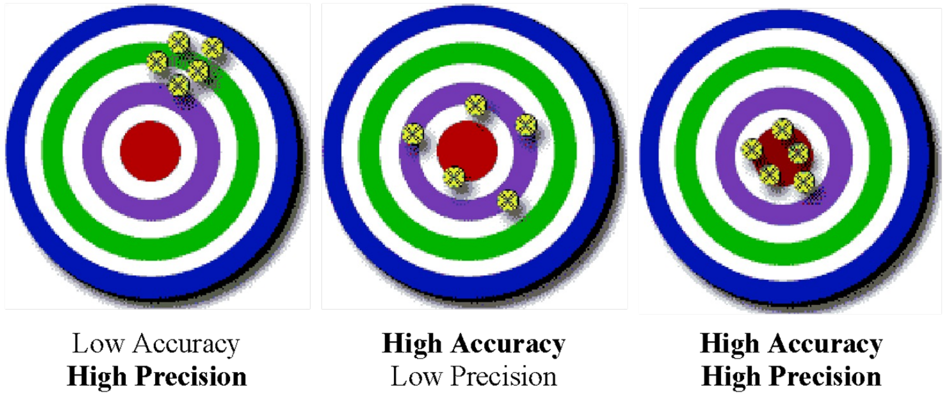
Important time markers (See also Section C-4 of WMO/GAW Report No. 268) are:

- Time stamp ($\boldsymbol{t_{UTC,\ IB1}}$) in UTC of the measurement of I_{B1} (background current after ozone exposure) during preparation. During pre-launch the Flight Time $\mathbf{t_{F,\ Pre\text{-}launch}}$ **< 0 seconds**
- Time stamp of the launch ($\boldsymbol{t_{UTC,\ Launch}}$) in UTC; here the flight time $\mathbf{t_{F,Launch}}$ **= 0 seconds**
- Time stamp of the balloon burst ($\boldsymbol{t_{UTC,\ Burst}}$) in UTC

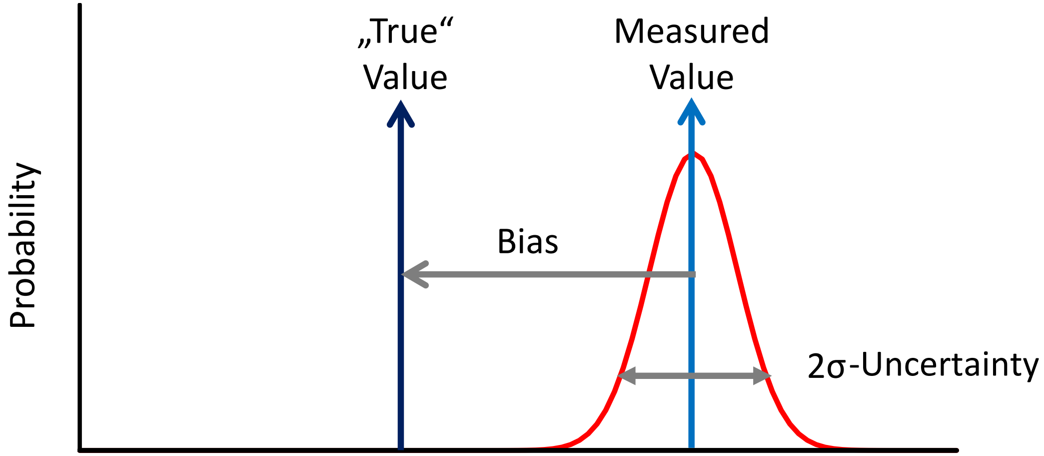
UTC = Coordinated Universal Time = GMT = Greenwich Mean Time

Precison, Accuracy, Bias and Uncertainty Budget *(Section C-2 GAW No.268)*

Precision and Accuracy



Bias and Uncertainty



Uncertainty Budget Ozonesonde Equation: E-3-1

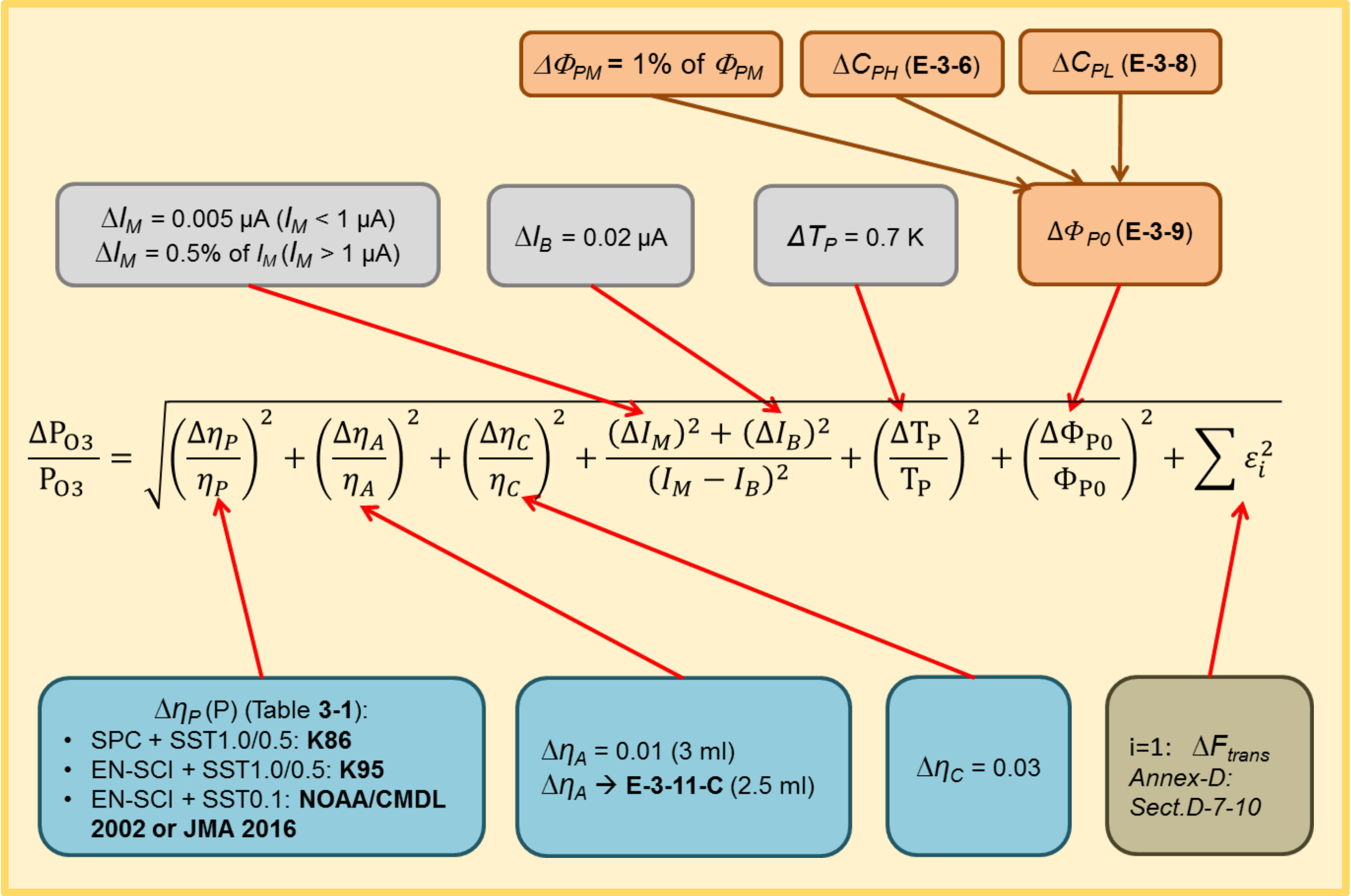
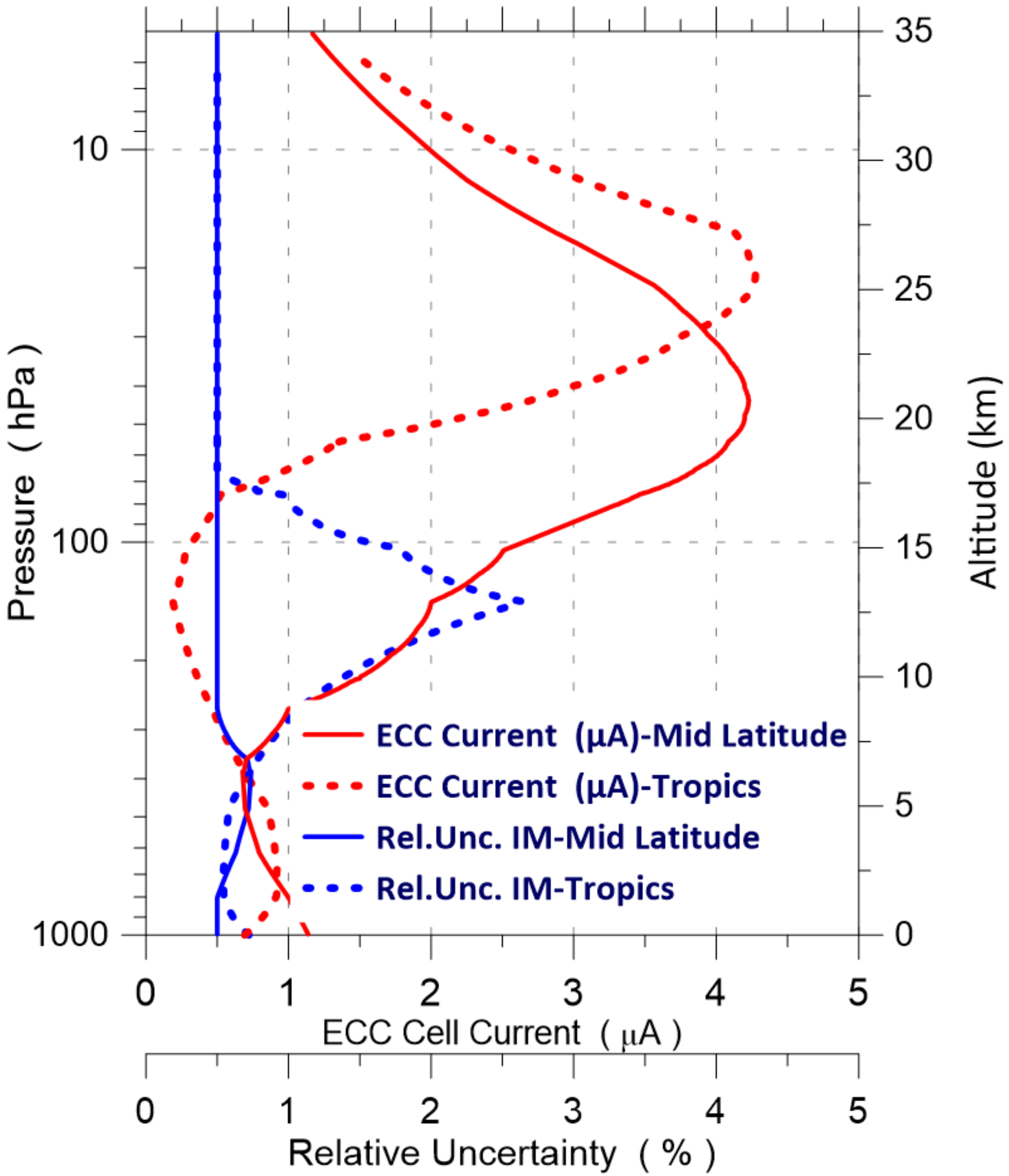


Figure C-4 of Annex-C of GAW No.268

See Also Section 3.3.1 of GAW Report No. 268

Measured Cell Current: I_M & its Uncertainty ΔI_M *(Section C-6.2)*



$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P * \eta_A * \eta_C * \Phi_{P0})} * (I_M - I_B)$$

The uncertainty of the measured sensor current (I_M) is mainly determined by the uncertainty of the current measurement made by the electronics (current to voltage converter) of the sonde data interface board, which is for modern interfaces:

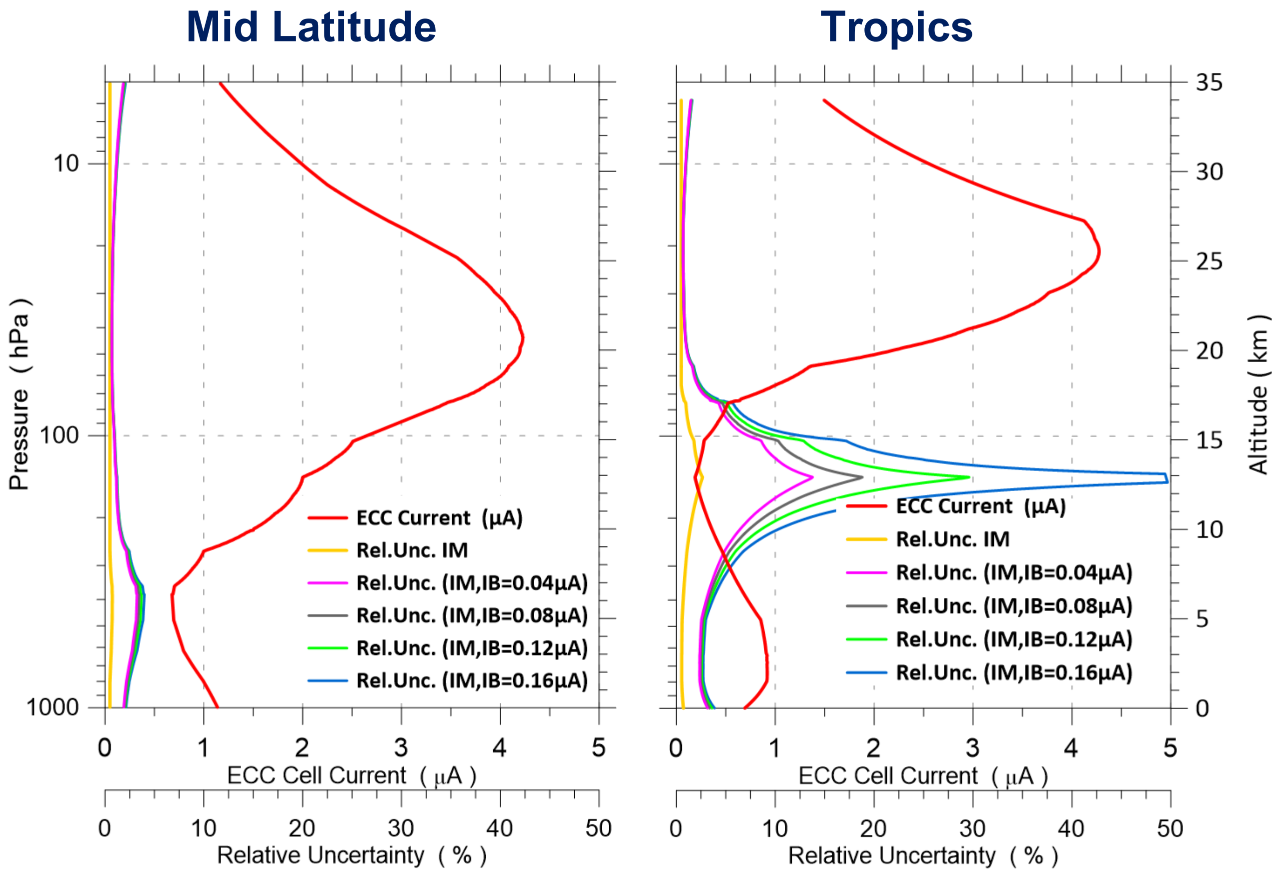
(**Section 3.3.6 of WMO/GAW No. 268**)

$\Delta I_M = \pm\ 0.005\ \mu A$ at $I_M < 1.00 \mu A$

$\Delta I_M = \pm\ 0.5\%$ of I_M at $I_M > 1.00 \mu A$

Background Current: I_B & its Uncertainty ΔI_B *(Section C-6.3)*

$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P * \eta_A * \eta_C * \Phi_{P0})} * (I_M - I_B)$$



Following the recommendations in **Section 3.3.6 of GAW No. 268,** the following background current correction is to be applied:

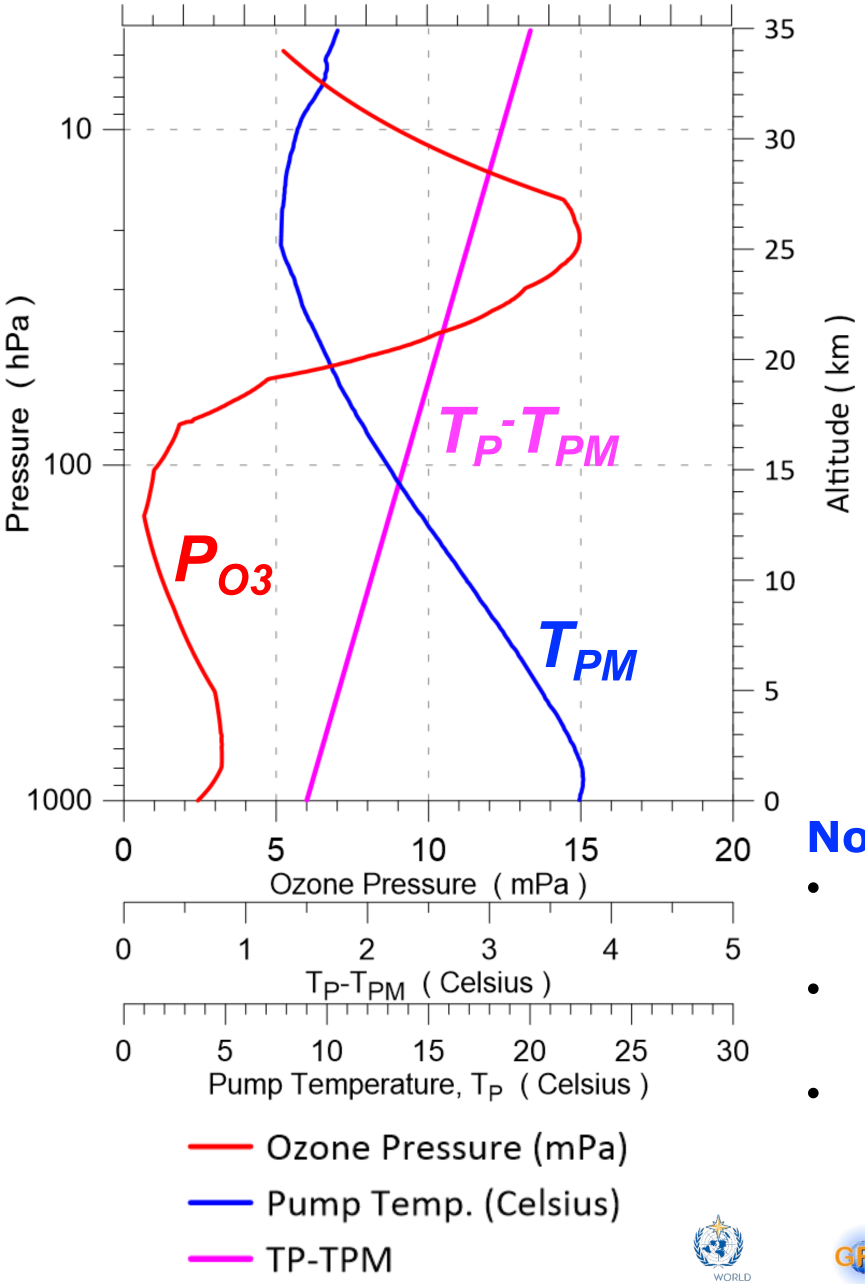
I. ***I_B = I_{B1},*** i.e. the background current measured 10 min. after the ECC sonde has been exposed to a dose of ozone at a cell current of about 5 μA for 10 min.

II. **Constant** through the entire sounding profile (i.e. independent of air pressure)

III. ***ΔI_{B1}* = ± 0.02 μA** in case of a proper background measurement (***I_{B1}*** < 0.07 μA)

- The ASOPOS panel has abandoned the further recording and processing of ***I_{B2}*** (after exposure of ozone, just prior to launch) as described in Section 3.3.6 of WMO/GAW No. 268.
- Therefore, the panel recommends the use of ***I_{B1}*** in formula E-2-1 (See ASOPOS-Webinar No. 3 on SOP's)

Pump temperature (in-flight): T_P & its Uncertainty ΔT_P *(Section C-6-4)*



$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P * \eta_A * \eta_C * \Phi_{P0})} * (I_M - I_B)$$

The (internal) pump temperature T_{PM} measured by a thermistor in a hole drilled into the Teflon block of the pump has to be corrected in order to approach the best representative pump temperature T_P *(Section 3.3.8 of WM/GAW No. 268)* by applying **Eq. E-3–15**:

$$T_P = T_{PM} + 3.90 - 0.80 * Log_{10}(P_{air})$$

The corresponding overall uncertainty ΔT_P **= 0.7 K** ⇨ $\frac{\Delta T_P}{T_P} \approx 0.3\%$

Note:

- Before 1996 the pump temperature was measured externally (box, taped at inlet or outlet of the pump tubes, or on the metal frame of the ECC-sensor).
- These measured temperatures could be 1-8 °C lower than the internal pump temperature.
- Pressure dependent correction formulas have been developed to correct for these artefacts (See Annex D of the WMO/GAW No.268 Report)

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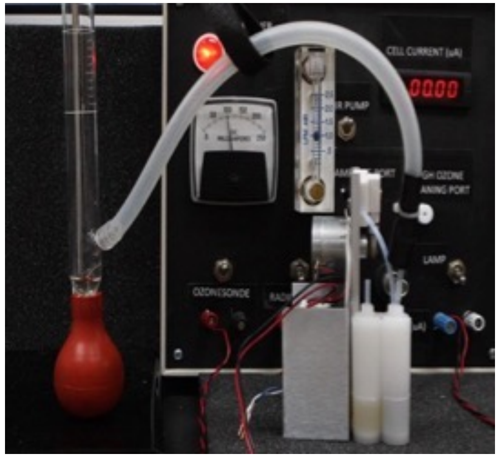
Pump flowrate at ground (preparation): Φ_{PM} & uncertainty $\Delta\ \Phi_{PM}$ *(Section C-6.1)*

$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P*\eta_A*\eta_C*\Phi_{P0})} * (I_M - I_B)$$



The pump flowrate Φ_{PM} (in ml/sec) as measured with a bubble flow meter at the gas outlet of the sensing cathode cell:

$$\Phi_{PM} = \frac{100}{t_{100}} \qquad \text{[E-3–2]}$$

t_{100} = time (seconds) measured for a bubble to pass through 100 ml of volume of the meter.

The uncertainty $\Delta\Phi_{PM}$ = ***1 %*** of measured value Φ_{PM}.

(same uncertainty also for well maintained and calibrated automated commercial flowmeters)

The measured flowrate Φ_{PM} has to be corrected for:

1. **Temperature effect**: small decrease in flowrate by factor C_{PL} through the slightly enhanced pump temperature T_P inside the Teflon pump base of about 2 K compared to laboratory temperature T_{Lab}
2. **Humidification effect :** increase of flowrate by factor C_{PH} due to evaporation of liquid in the cathode cell and bubble flowmeter

Corrected Pump flowrate at ground: Φ_{P0} & its Uncertainty $\Delta\ \Phi_{P0}$ *(Section C-6.1)*

$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P * \eta_A * \eta_C * \Phi_{P0})} * (I_M - I_B)$$

The measured flowrate Φ_{PM} has to be corrected for:

1. Temperature effect: small decrease in flowrate by factor C_{PL} through the slightly enhanced temperature inside the Teflon pump base of about 2 K compared to laboratory temperature T_{Lab}
2. Humidification effect : increase of flowrate by factor C_{PH} due to evaporation in the cathode cell and the bubble flowmeter.

The corrected pump flow rate Φ_{P0} at ground is

$$\Phi_{P0} = (1 + C_{PL} - C_{PH}) * \Phi_{PM} \quad \textbf{(E-3-3)}$$

1. Temperature correction C_{PL}

$$C_{PL} = \frac{T_P - T_{Lab}}{T_{Lab}} \text{ and } T_P - T_{Lab} \cong 2K \quad \textbf{(E-3-7)}$$

$$C_{PL} = 0.007$$

And its uncertainty ΔC_{PL}

$$\Delta C_{PL} = \frac{\Delta T_{PI}}{T_{Lab}} \cong \frac{0.5}{T_{Lab}} \cong 0.007 \quad \textbf{(E-3-8)}$$

2. Humidification correction C_{PH}

$$C_{PH} = \left(1 - \frac{RH_{in}}{100}\right) \cdot \frac{e_{sat}(T_{Lab})}{P_{Lab}} \quad \textbf{(E-3–4)}$$

And its uncertainty ΔC_{PH}

$$\Delta C_{PH} = (C_{PH,High} - C_{PH,Low})/(2\sqrt{3}) \quad \textbf{(E-3–6)}$$

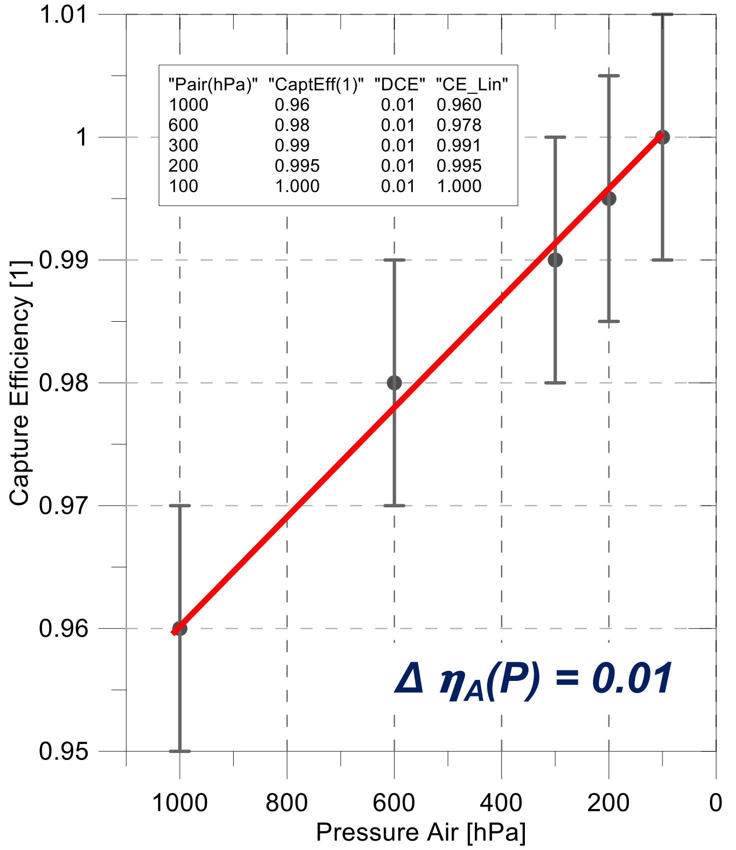
Typical C_{PH} and ΔC_{PH} values are:

- T_{Lab} = 20 ^{o}C: $C_{PH} \approx$ 0.01-0.02 and $\Delta C_{PH} \approx$ 0.003
- T_{Lab} = 30 ^{o}C: $C_{PH} \approx$ 0.02-0.04 and $\Delta C_{PH} \approx$ 0.005

Absorption Efficiency (empirical): $\eta_A(P)$ & its Uncertainty $\Delta\ \eta_A(P)$ *(Section C-6.5)*

$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P * \eta_A * \eta_C * \Phi_{P0})} * (I_M - I_B)$$

η_A(P) for cathode Cell charged with 2.5 cm3 solution



File: Capture Efficiency-V3.grf

- The absorption efficiency is the capture-efficiency that the sampled gaseous ozone is transferred into the aquous sensing solution in the cathode cell.
- Depending on the volume of the sensing solution in the cathode cell the following recommendations for the absorption efficiency η_A and its uncertainty η_A are made (Section 3.3.4 of WMO/GAW No.268):

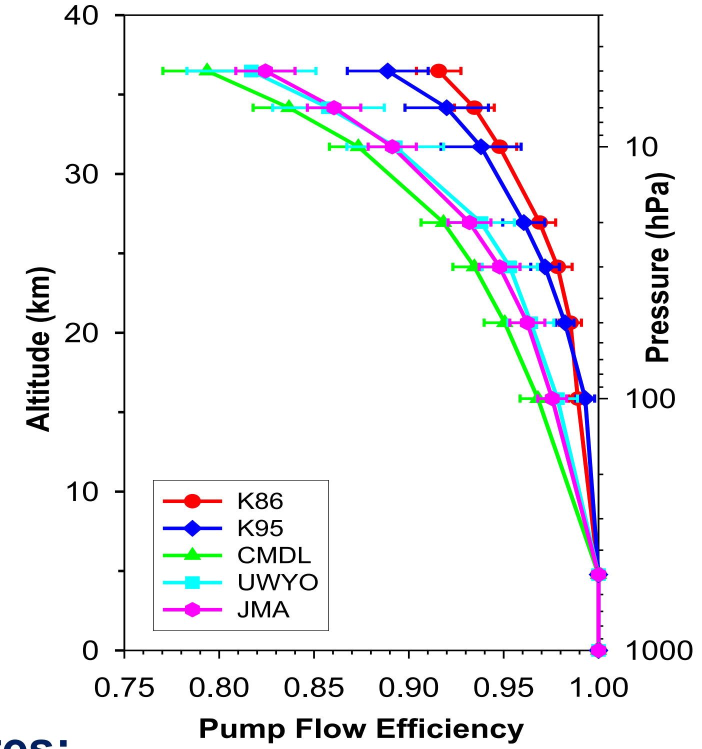
  1) Cathode cells charged with 3.0 cm^3 of cathode solution

  $$\eta_A = 1.00 \quad \& \quad \Delta\eta_A = 0.01$$

  2) Cathode cells charged with 2.5 cm^3 of solution require a small correction as a function of ambient air pressure P_{Air}. *For details see Section 3.3.4.*

Pump Efficiency: $\eta_P(P)$ & its Uncertainty $\Delta\,\eta_P(P)$ *(Section C-6.6 of GAW No.268)*

$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P * \eta_A * \eta_C * \Phi_{P0})} * (I_M - I_B)$$



At ambient air pressures lower than 100 hPa the efficiency of the gas sampling pump degrades as a function of ambient pressure. Depending on the sonde and sensing solution type, these recommended efficiency tables should be used (Section 3.3.3 of WMO/GAW No.268):

a. **Komhyr-1986 (K86-Efficiency) for SPC-6A sondes with SST1.0 or SST0.5;**

b. **Komhyr-1995 (K95-Efficiency) for ENSCI sondes with SST1.0 or SST0.5;**

c. **Johnson-2002 (CMDL-Efficiency) or Nakano- 2019/2022 (JMA-Efficiency) for ENSCI sondes with SST0.1.**

Notes:

- The corresponding pressure dependent pump efficiencies η_P and their uncertainties $\Delta\eta_P$ as a function of ambient air pressure P_{Air} are listed in Table 3–1 (Section 3.3.3).
- Between 100 and 10 hPa Johnson-2002, Nakano-2019 and Nakano-2022 *(AMT, 2022)* agree within bette than 1% deviation

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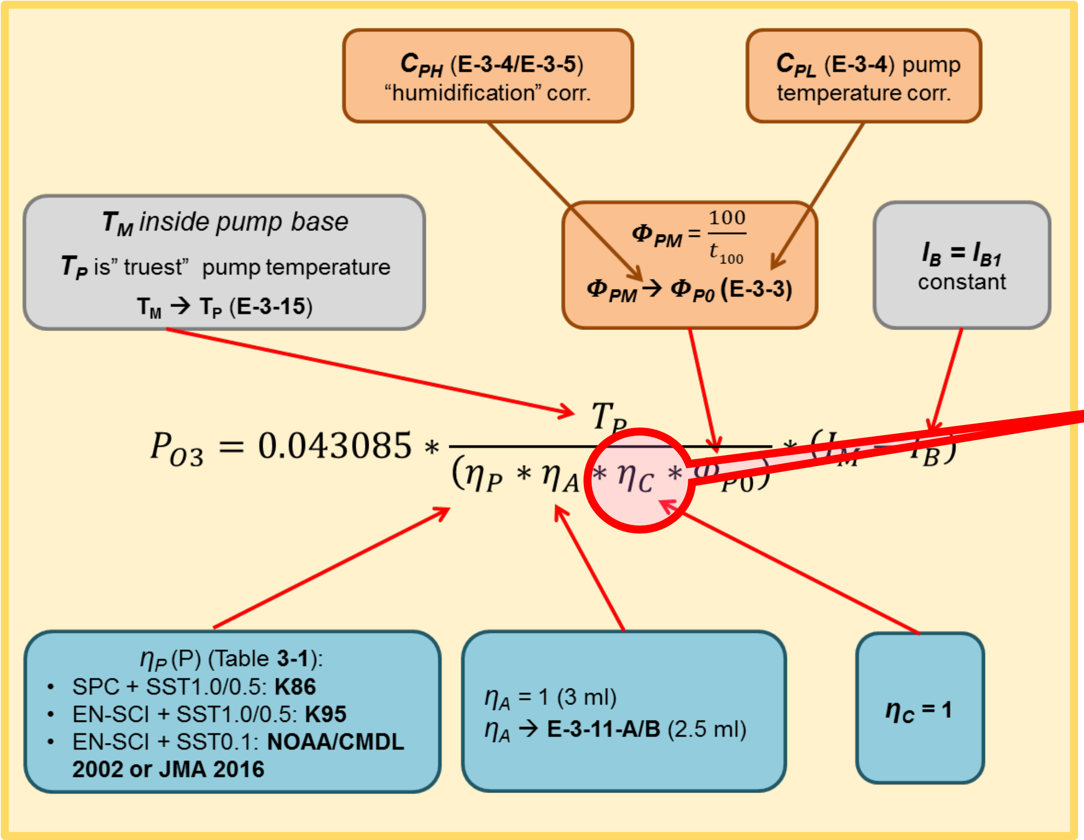
Conversion Efficiency (empirical): $\eta_C(P)$ & its Uncertainty $\Delta\,\eta_C(P)$ (Section C-6.7)

$$P_{O3} = 0.043085 * \frac{T_P}{(\eta_P*\eta_A*\eta_C*\Phi_{P0})} * (I_M - I_B)$$



In Section 3.3.5 of GAW No. 268, for the conversion efficiency $\eta_C(P)$ and its uncertainty $\Delta\eta_C(P)$, the following constant values are recommended:

$$\eta_C = 1.00 \qquad \textit{and} \qquad \Delta\eta_C = 0.03$$

Overall Uncertainty and its Uncertainty Budget *(Section 3.3.12 of GAW No.268)*

$$\frac{\Delta P_{O3}}{P_{O3}} = \sqrt{\left(\frac{\Delta\eta_P}{\eta_P}\right)^2 + \left(\frac{\Delta\eta_A}{\eta_A}\right)^2 + \left(\frac{\Delta\eta_C}{\eta_C}\right)^2 + \frac{(\Delta I_M)^2+(\Delta I_B)^2}{(I_M-I_B)^2} + \left(\frac{\Delta T_P}{T_P}\right)^2 + \left(\frac{\Delta\Phi_{P0}}{\Phi_{P0}}\right)^2 + \sum \varepsilon_i^2} \qquad \text{[E-3-1]}$$

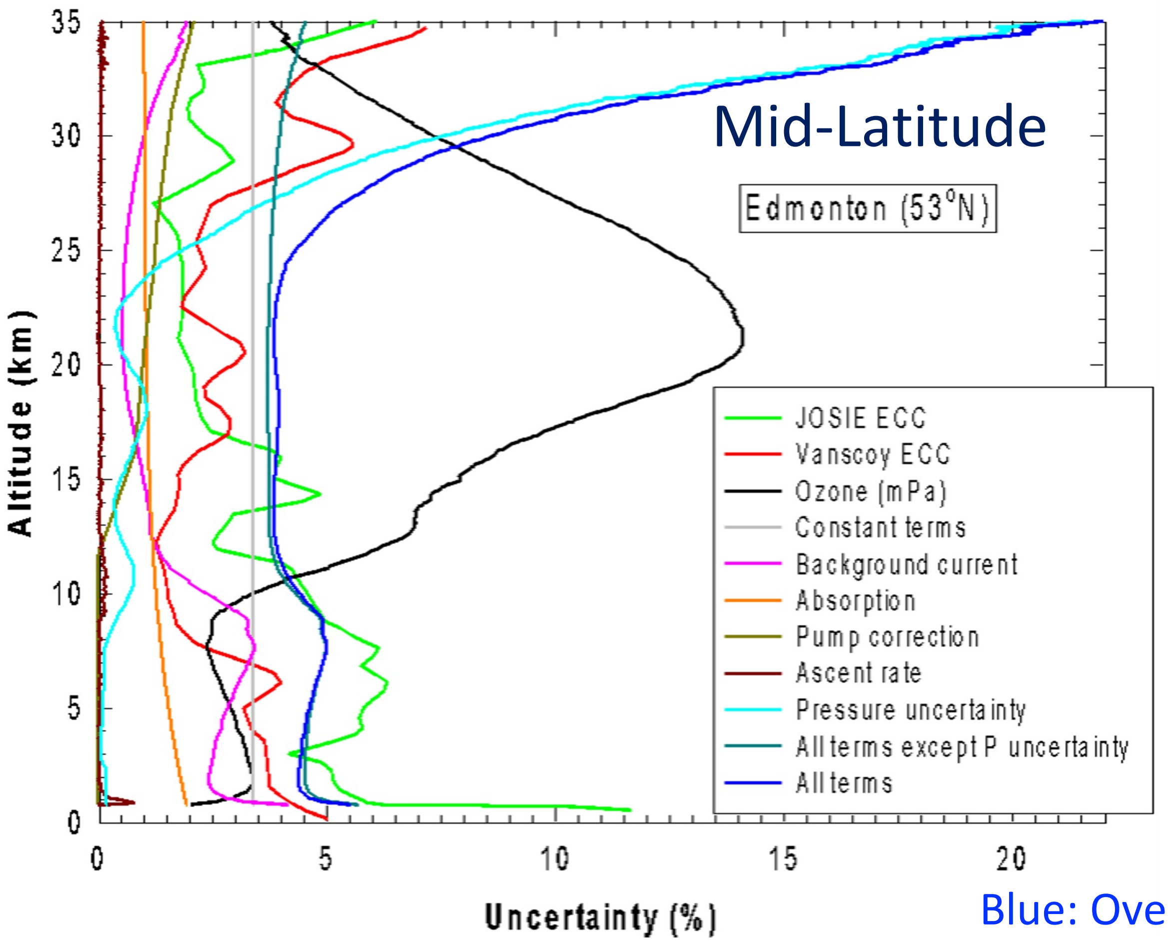


Figure 3-9 (Page 52 of GAW No. 268)

Blue: Overall Uncertainty

Pink: Background Current

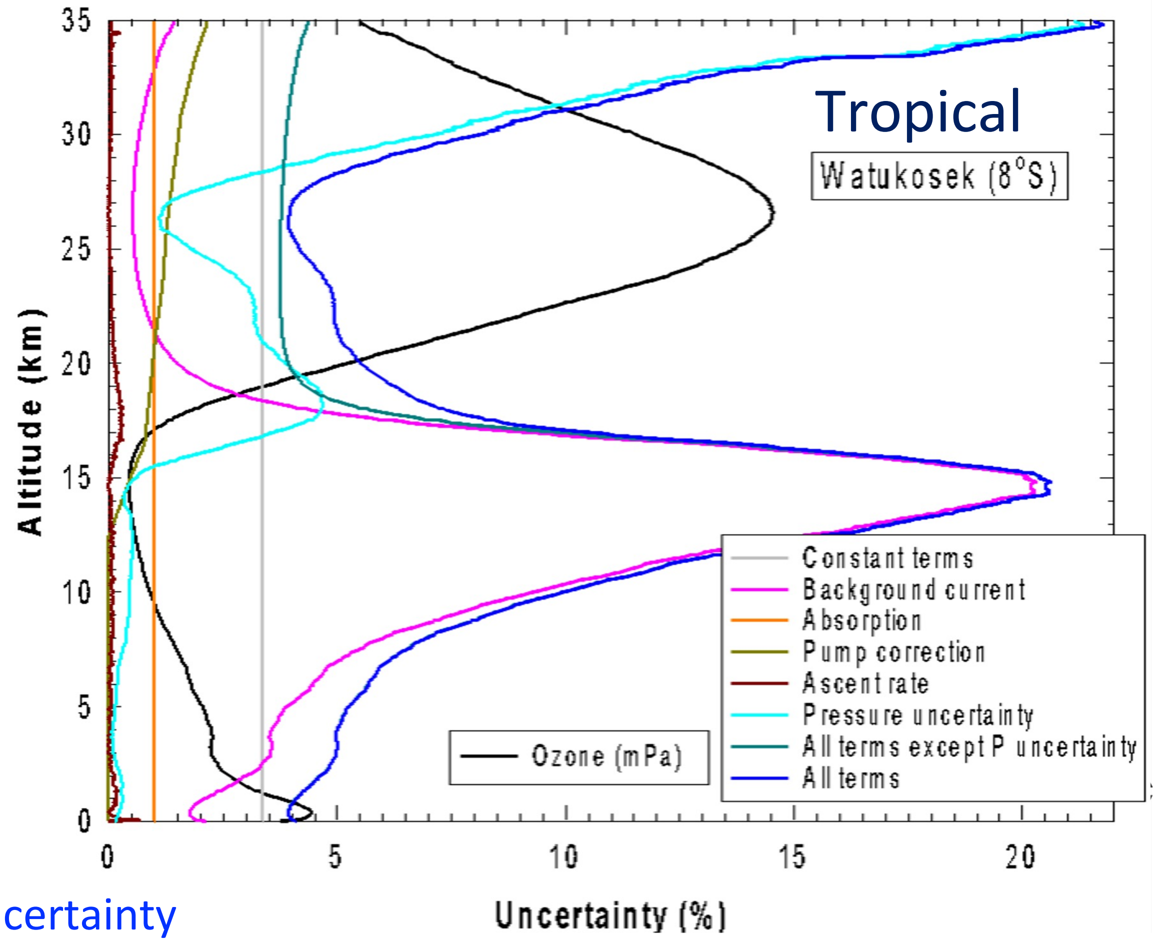


Figure 3-10 (Page 52 of GAW No. 268)

For details: Tarasick et al., 2021, https://doi.org/10.1029/2019EA000914

Data Processing: Key Points

- In ASOPOS 2.0 the data processing methodology to follow has remained the same as that formulated in ASOPOS 1.0 (GAW Report No. 201, 2014), with some important exceptions :
  - Background current $I_B = I_{B1}$ and NOT I_{B2} as previously recommended.
  - Corrections to the pump flowrate determined at the ground now include the pump temperature correction and the humidification correction.
  - Recommendation that for low buffered sensing solution (En-Sci SST0.1) the pressure dependent CMDL/JMA pumpflow efficiencies should be used.
- New in ASOPOS 2.0 are the practical guidelines to derive the different contributions to the instrumental uncertainty, to estimate the overall measurement uncertainty budget; these values are stored in the sonde data files.
- All the supporting data necessary to derive the ozone partial pressure and its uncertainties must be included in the metadata as essential information for data processing, as well as for possible future re-processing.
- ASOPOS 2.0 has established the scientific basis for future resolution of the slow and fast time response of the ECC ozone sensor.
- ASOPOS 2.0 also includes practical guidelines for the homogenisation of historical long term ozone records.

Closing Remarks

- This webinar no.4 is part of a series of six ASOPOS Webinars:
  1. Introduction to ASOPOS 2.0: An Overview *(Anne Thompson & Herman Smit)*
  2. Hardware *(Herman Smit & Roeland VanMalderen)*
  3. SOP: Standard Operating Procedures *(Roeland VanMalderen & Peter van der Gathen & Gary Morris & Bryan Johnson)*
  4. Data Processing *(Herman Smit & David Tarasick)*
  5. Data Quality Indicators (DQI) *(Ryan Staufer & Holger Voemel)*
  6. Meta Data and Software *(Ryan Staufer & Roeland VanMalderen)*
- The webinars do not replace the report or associated video clips, but only highlight the most important topics and changes with respect to the previous ASOPOS 1.0 report (GAW Report No. 201, 2014).
- **For questions, clarification or general advice, the authors of this webinar and the ASOPOS Team are more than happy to assist!!!**

Thank you for your attention and for good collaboration in the future !!!

Back Up Slides

Pump Efficiency (PFE): $\eta_P(P)$ & its Uncertainty $\Delta\ \eta_P(P)$ (2)

- Addendum Nov.2022: New PFE-Publication by Nakano and Morofuji in AMTD giving new PFE values and their uncertainties, obtained over all 1387 PFE Samples they obtained in period 2009-2022. *https://doi.org/10.5194/egusphere-2022-565*
- Between 100 and 10 hPa Nakano-2019 and Nakano-2022 agree within better than 1% deviation

Expanded Table 3-1 (Section 3.3.3) of pressure dependent pump efficiencies η_P and their uncertainties $\Delta\eta_P$ as a function of ambient air pressure P_{Air}

Pressure [hPa]	ECC (SPC-6a) Komhyr,1986 K86-Efficiency	ECC (ENSCI) Komhyr et al., 1995 K95-Efficiency	ECC (CMDL) Johnson et al., 2002	ECC (UWYO) Johnson et al., 2002	ECC (JMA) Nakano, 2019	ECC (JMA*) Nakano et al., 2022
1000	1	1	1	1	1	1
100	0.989 ± 0.005	0.993 ± 0.005	0.968 ± 0.009	0.978 ± 0.011	0.976 ± 0.008	0.978 ± 0.009
50	0.985 ± 0.006	0.982 ± 0.005	0.951 ± 0.011	0.964 ± 0.012	0.962 ± 0.009	0.964 ± 0.011
30	0.978 ± 0.008	0.972 ± 0.008	0.935 ± 0.011	0.953 ± 0.015	0.948 ± 0.011	0.948 ± 0.013
20	0.969 ± 0.008	0.961 ± 0.011	0.918 ± 0.012	0.938 ± 0.018	0.932 ± 0.011	0.929± 0.014
10	0.948 ± 0.009	0.938 ± 0.021	0.873 ± 0.015	0.893 ± 0.026	0.891 ± 0.013	0.883 ± 0.017
7	0.935 ± 0.010	0.920 ± 0.022	0.837 ± 0.019	0.858 ± 0.029	0.861 ± 0.014	0.848 ± 0.020
5	0.916 ± 0.012	0.889 ± 0.021	0.794 ± 0.023	0.817 ± 0.034	0.824 ± 0.016	0.807 ± 0.023