830 Douglas Ave.
Dunedin, FL 34698
(727)733-2447
Fax:(727)733-3962
www.OceanOptics.com

Engineering Note

Topic: NeoFox Calibration and Measurement

Products Affected: NeoFox

Date Issued: 04/18/2011

Algorithms

Overview

NeoFox is a dynamic measurement system that has been designed to work with a variety of optical probes to measure oxygen. To support the various probe technologies and the broad spectrum of applications that employ the system, the NeoFox measurement system supports a number of configuration options. This document defines the algorithms by which the NeoFox system produces its measurements, the various configuration options required to implement these algorithms, and the ways in which those configuration options can be exercised.

Below is the process by which the NeoFox measurement system produces its oxygen values. Details regarding each step follow in the next section.

1. The chemistry's tau value is measured by the hardware.
2. Tau is converted to percent oxygen.
3. Percent oxygen is converted to converted oxygen.

Detailed Algorithm Description

Step 1 – Calculating the chemistry's tau:
The NeoFox hardware optically stimulates and measures the fluorescent decay rate of the probe's chemicals. The fluorescent decay rate of the chemistry is sensitive to both the temperature and the partial pressure of oxygen in its ambient environment. The output of the hardware's measurement of the decay rate is a variable known as "tau". It is important to note that although tau is correlated to the decay lifetime, it is not an actual measurement of the lifetime itself and should not be used as such.

Step 2 – Converting from tau to percent oxygen:

Because tau is a function of the chemistry's response to the partial pressure of oxygen and temperature, it is possible to invert this relationship and calculate the partial pressure of oxygen from known values of tau and temperature. The output of the conversion is a partial pressure, expressed as percent of 1 ATM. This is the variable known as "percent oxygen". It is extremely important to note that this percent oxygen measurement is NOT a percent of ambient pressure measurement. Pressure from other gasses will not affect the percent oxygen measurement.

There are two potential methods for converting from tau to oxygen: the "two-point conversion" and the "multipoint conversion". The major difference between these two methods is that the two-point conversion does not consider temperature when calculating the partial pressure of oxygen from tau, but the multipoint conversion does. Hence, while multipoint conversion is more accurate than two-point conversion, the two-point conversion is simpler to implement and less expensive.

For more information on the conversion methods, see ***Conversion** from Tau to **Oxygen:** Two-Point Conversion* and ***Conversion** from Tau to **Oxygen: Multipoint** Conversion*.

Step 3 – Converting from "percent oxygen" to "converted oxygen"

Once the partial pressure of oxygen has been calculated as a percentage of 1 ATM, this percent oxygen may be converted into different units in a variable called "converted oxygen". This conversion can also be used to convert from oxygen partial pressure to dissolved oxygen concentration.

For more information on converting from percent oxygen to converted oxygen, see ***Conversion** to Alternate Oxygen **Units***.

Conversion from Tau to Oxygen: Two-Point Conversion

Two-point conversion is the simplest, but less accurate, of the two methods that can be used to convert from tau to oxygen. A two-point calibration uses two samples of oxygen-tau pairs to approximate a linear relationship between the reciprocal of tau and oxygen. Generally, ambient air is used as one of the two reference points, since its percent oxygen can be reliably assumed to be 20.9% of 1 ATM. The second point must be a sample taken at 0% oxygen. Once the tau values at these two points have been measured, the offset, slope, and tau0 values are calculated and downloaded to the device, where the conversion will be performed according to the following formula.

```
PO2 = A + B • TAU0 / TAU
```

- `PO2 is "percent oxygen"`
- `A is the two point calibration offset`
- `B is the two point calibration slope`
- `TAU0 is the tau value observed at a known condition of 0% oxygen.`
- `TAU is the tau value produced by the chemistry`

The reduced accuracy of the two-point conversion is due to two factors. Most obviously, because it uses just 2 points in its calibration, the tau0/tau vs oxygen curve fit is approximated as a straight line instead of a parabolic curve, which is the actual shape of the calibration relationship between tau0/tau and oxygen.

More significantly, the two-point conversion method does not account for the contribution of temperature to tau. Therefore, two point conversions are generally recommended only in cases where the temperature is unlikely to differ from the calibration temperature and a high degree of accuracy is not needed.

Conversion from Tau to Oxygen: Multipoint Conversion

The multipoint conversion method requires a more complex calibration, but is more accurate than the two-point method. The multipoint method also accounts for the effect of temperature on tau, and therefore is suitable for use in situations where temperature may change over the course of an experiment.

In a multipoint calibration, many samples are taken over the applicable measurement range. Each sample consists of three known values: tau, temperature, and oxygen (in percent of 1 ATM). These samples are then curve fit with second order polynomial approximations to produce the conversion formulas that follow.

```
AA = TEMP • TEMP • A0 + TEMP • A1 + A2
BB = TEMP • TEMP • B0 + TEMP • B1 + B2
CC = TEMP • TEMP • C0 + TEMP • C1 + C2
TT = TEMP • TEMP • T0 + TEMP • T1 + T2

PO2 = TT/TAU • TT/TAU • AA + TT/TAU • BB + CC;
```

- AA, BB, CC, TT are the temperature dependant coefficients for the final oxygen conversion equation
- A0, A1, A2, B0, B1, B2, C0, C1, C2, T0, T1, T2 are the constants for the temperature dependant coefficient equations.
- TEMP is the temperature, in Kelvin
- TAU is the "tau" value produced by the chemistry
- PO2 is "percent oxygen"

As shown above, the conversion algorithm essentially works in two steps. The second of the two steps is a fairly straightforward second order equation that computes "percent oxygen" as a function of Tau from 4 coefficients (TT, AA, BB, CC) and does not account for temperature. The temperature compensation is provided by the temperature sensitivity of the coefficients themselves : hence, the need for the first step, which computes each of the four coefficients as a function of temperature.

In-Field Calibration Reset

Although the main calibration itself can be performed just once, in a controlled laboratory environment, it is important to perform an in-field recalibration prior to beginning any experiments. The need for in-field recalibration applies to both the two point and the multipoint calibration options, although each calibration method requires a different recalibration procedure.

Two Point Calibration In-Field Recalibration

The process for recalibrating the two-point conversion constants is essentially the same as the original calibration process, in which two points are used to calculate slope, offset, and tau0. However, during an in-field recalibration, only the non-zero oxygen pressure point (usually 20.9% oxygen) is re-sampled. The original 0% oxygen sample is then used with the new non-zero reference point and the two point calibration procedure is repeated.

Multi Point Calibration In-Field Recalibration

The process for recalibrating the multipoint conversion constants is known as a "single point reset". In a single point reset, a new temperature-tau-oxygen point is sampled (usually ambient conditions) and then this new reference point is used to adjust the calibration curves to fit this point. The adjustment is made by using the known values of oxygen, tau, and temperature to solve the original multi point calibration equations for a new value of the T2 constant.

```
AA = TEMP • TEMP • A0 + TEMP • A1 + A2
BB = TEMP • TEMP • B0 + TEMP • B1 + B2
CC = TEMP • TEMP • C0 + TEMP • C1 + C2
TT = TEMP • TEMP • T0 + TEMP • T1 + T2

[This step solves the multipoint O2 eqn for TT/TAU]
[PO2 = TT/TAU • TT/TAU • AA + TT/TAU • BB + CC]
NEW_TT_TAU1 = (-BB + √(B² -4•AA•(CC-PO2)))/(2 • AA)
NEW_TT_TAU2 = (-BB - √(B² -4•AA•(CC-P02)))/(2 • AA)
NEW_TT_TAU  = NEW_TT_TAU1 when NEW_TT_TAU1 ≥ 0
              |NEW_TT_TAU2| when NEWTT_TAU1 < 0

[This step calculates the new T2 coefficient]
NEW_T2 = T2 – (TT – NEW_TT_TAU • TAU)
```

- AA, BB, CC, TT are the original temperature dependant coefficients for the final oxygen conversion equation
- A0, A1, A2, B0, B1, B2, C0, C1, C2, T0, T1, T2 are the original constants for the temperature dependant coefficient equations.
- TEMP is the single point reset temperature, in Kelvin
- TAU is the single point reset tau value, in microseconds
- PO2 is the single point reset percent oxygen value.
- NEW_TT_TAU represents the new value of TT/TAU
- NEW_T2 is the new value of the T2 coefficient

Conversion to Alternate Oxygen Units

Currently, the following units are supported with the following conversion formulas. The concentration conversions are dependent upon temperature. To use a concentration conversion, you must have a temperature sensor or must manually provide a temperature.

1. % - Partial Pressure

```
[%] = PO2
```

- PO2 is "percent oxygen", as described above

2. ppm - Dissolved Concentration

$$[PPM] = e^{A1+A2\cdot T1+A3\cdot \ln(T2)+A4\cdot T2+SC\cdot (B1+B2\cdot T2+B3\cdot T2\cdot T2)} \cdot C \cdot PO2/D$$

- A1,A2,A3,A4,B1,B2,B3,C,D are constants, hardcoded in the firmware.
- T1 is 100 divided by the temperature (in Kelvin).
- T2 is the temperature (in Kelvin) divided by 100.
- SC is the "salinity correction factor", which can be set by software:

```
A1   -173.9894
A2    255.5907
A3    146.4813
A4   - 22.204
B1   -  0.037362
B2      0.016504
B3   -  0.0020564
C       0.032
D      20.9
```

- PO2 is the "percent oxygen", as described above.

3. Torr – Partial Pressure

```
[TORR] = PO2 / 100 * 760
```

- PO2 is "percent oxygen", as described above

4. umol/L – Dissolved Concentration

```
[UMOL/L] = 1000 / 31 • PPM
```

- PO2 is "percent oxygen", as described above
- PPM is the converted PPM value, as described above

Temperature Sources

The temperature value used in the conversion algorithms can come from any of the following three sources:

- The temperature sensor attached to the NeoFox
- A manually user-entered temperature value, or
- No temperature value at all

The temperature source can be set in the calibration screen of the NeoFox Viewer. It is important to note that even though the temperature values are generally displayed and set in degrees Celsius, they are implemented as degrees Kelvin in the algorithms.