parSYNC® PLUS

Gas and Particulate Matter Sensors – Technical Overview

August 3, 2022

DRAFT

Table of Contents

Introduction

This document covers the equations and working principles for the gas and particulate matter (PM) sensors in the parSYNC PLUS (pS+). For gases, the pS+ measures carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxide (NO), and nitrogen dioxide (NO_2) concentrations. For PM, the pS+ uses three sensor types – ionization, scattering, and opacity – to report particle mass (PM) and particle number (PN) concentrations. The pS+ is also called parSYNC 3.8 (pS3.8) in some documents.

The latest model, parSYNC FLEX (pS-FLEX or FLEX), has additional sensors for gases, namely hydrocarbon (HC and oxygen (O_2). The information in this document is applicable to the FLEX with some minor exceptions. A separate document specific to the FLEX will soon be released.

Equations to Calculate Concentration

This section describes the system of equations that are used in the parSYNC® to interpret the voltage or current electrical response from the sensor to a concentration value for a gas molecule or particulate matter in the exhaust sample. The electrical signals are acquired at 100 hz, averaged over a 1 second duration to produce a 1 hz electrical signal, which is converted to a 1 hz concentration value using the equations described here.
100 hz electrical signal data acquisition ➔ 1 hz electrical signal ➔ 1 hz concentration value

Equations for Gas Sensors

$$V_i = V_r - V_z$$

$$C_i = V_i * \frac{C_s - C_z}{V_s - V_z} + C_z$$

Where,

- C_i instantaneous, zero corrected, concentration of measured gas, ppm or %
- C_s specified concentration of span gas, ppm or % (*GUI name: Span Conc.*)
- C_z specified concentration of zero gas, ppm or % (typically zero). If using clean ambient air, CO_2 in atmosphere is not zero. Global average CO_2 in 2022 is ~410 ppm (0.041%). (GUI name: Zero Conc.).
- V_i instantaneous, zero corrected, sensor voltage, V
- V_r instantaneous, raw, sensor voltage, V. *When sampling zero gas, ideally, $V_r = V_z$ and thus V_i = 0V and C_i=0. But, in reality, $V_r \sim V_z$, and so V_i and C_i are ~ 0.*
- V_s average of instantaneous raw voltage when sampling span gas, V (*GUI name: Span Vraw*)
- V_z average of instantaneous raw voltage when sampling zero gas, V (*GUI name: Zero Vraw*)

Equations for PM Sensors

Step-1
Calculate PM (µg/m^3) and particle number, PN (#/cm^3) for **each** sensor as per:

Sensor	V_i	*PM (µg/m3)*	*PN (#/cm3)*
Scattering	$V_r - V_z$	$a*V_i^2 + b*V_i$	$x* V_i^2 + y*V_i$
Ionization	$-(V_r - V_z)$	$a*V_i^2 + b*V_i$	$x* V_i^2 + y*V_i$
Opacity	$-(V_r - V_z)$	$a*V_i^2 + b*V_i$	$x* V_i^2 + y*V_i$

For ionization and opacity sensors, the V_i equation has a negative sign because the raw voltages are inversely proportional to particulate matter concentration.

Where,

- a,b coefficients for each sensor for PM. *User can change these in the GUI.*
- V_i instantaneous, zero corrected, sensor voltage, V. *Written as NA during zeroing.*
- V_r instantaneous, raw, sensor voltage, V. *When sampling zero gas, ideally, $V_r=V_z$ and thus $V_i=0V$, and subsequently PM=0 and PN=0. But, in reality, $V_r \sim V_z$, and so Vi, PM, and PN are ~ 0.*
- V_z average of instantaneous raw voltage when sampling zero gas, V (*GUI name: Zero Vraw*)
- x,y coefficients for each sensor for PN. *User can change these in the GUI.*

Step-2

The final PM (µg/m^3) and PN (#/cm^3) reported in the data file are a weighted sum of the PM (µg/m^3) and PN (#/cm^3), respectively, calculated for each sensor. Individual sensor PM and PN are neither displayed in the GUI nor recorded in the data file, however, the user can calculate these during post-processing using the equations described here and the config file used during measurement.

The "weight" is the fractional contribution of the individual sensor result to final reported concentration. User can change these values in the GUI. For each sensor, the weight can be minimum = 0.000 and maximum = 1.000. The sum of individual sensor weights must be 1.000. Set the weight for a sensor to zero to remove its contribution.

Coefficients and Weighs for PM (µg/m^3)

Sensor	'a'	'b'	Weight
Scattering	6534200	375640	0.550
Ionization	-948.97	6319.9	0.390
Opacity	269670	28252	0.060

Coefficients and Weighs for PN (#/cm^3)

Sensor	'x'	'y'	Weight
Scattering	3.8983E+9	8.8042E+8	0.010
Ionization	-2.744E+6	1.4262E+7	0.860
Opacity	2.9964E+8	7.6699E+7	0.130

Notes

1. Recorded in the data file and displayed on GUI: V_i and V_r for individual gas and particulate. sensors, and C_i for each gas sensor but only the final *PM* and *PN* value. During zeroing, V_i, C_i, *PM*, and *PN* are reported as NA.
2. Only displayed on GUI: C_s, C_z, V_s, V_z, and *PM* and *PN* coefficients and weights.

Overview of the Gas Sensors

The pS+ measures CO_2, CO, NO, and NO_2 gases. The latest model, parSYNC FLEX, also measures HC and O_2 and these are greyed out here to convey that they are unavailable in the pS+ model.

Measurement principle
CO_2, CO, HC: 3-channel non-dispersive infra-red (NDIR)
NO, NO_2, O_2: electro-chemical (EC), also known as micro-fuel cell

Specifications of the gas sensors

Parameter		CO_2	CO	HC	NO	NO_2	O_2
Range		0–20 %	0–15 %	0–4000 ppm	0–5000 ppm	0–300 ppm	0–100 %
$T_{0\text{-}90}$ Time (s)		< 3.5	< 3.5	< 3.5	< 5	< 35	< 6
Accuracy	Abs	± 0.3 %	± 0.02 %	± 8 ppm			± 0.1 %
	Rel	± 3 %	± 3 %	± 3 %			± 2 %
Resolution					1–2 ppm	0.1 ppm	
Repeatability	Abs	± 0.1 %	± 0.02 %	± 6 ppm			± 0.1 %
	Rel	± 2 %	± 2 %	± 2 %	± 2 %	± 2 %	± 2 %

This document will be updated to add basic working principles for NDIR and ECC. In the meantime, working principles of NDIR and ECC are easily found using a simple internet search. The pS+ NDIR has three measurement channels plus one reference channel. Thus, it has a four-window chopper. The NO and NO_2 sensors are 3-electrode ECs.

Overview of the PM Sensors

The parSYNC device uses three different types of sensors to determine particle mass and particle number. Each sensor is sensitive to different ranges of particle sizes and can measure the particle throughput in real-time. A multi-plex approach is used to combine data from the three sensors and provide the user with particle mass and particle number.

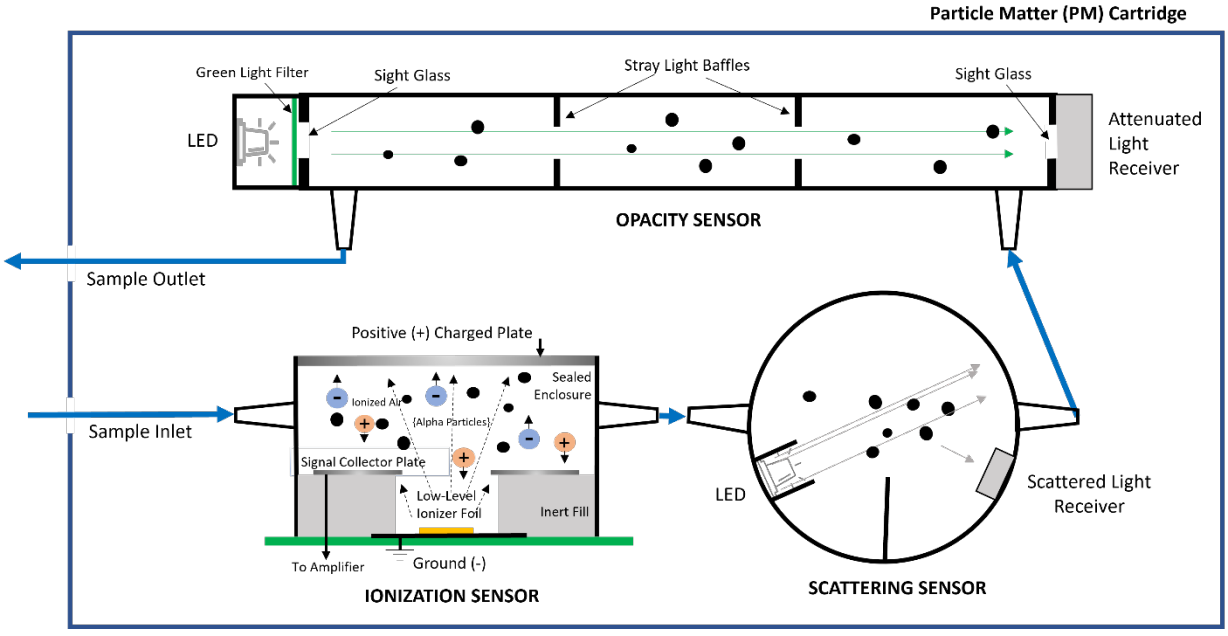
The parSYNC measures undiluted emissions using the response of three dissimilar particulate sensors. The sensors are sensitive to different distributions of particle size:

Sensor	Greatest Sensitivity
Ionization	Ultra-fine/Fine particulates, typically 0.01 to 0.3+ microns
Opacity	Overall particulates, typically 0.1 to 10+ microns, peak@0.8microns
Scattering	Coarse particulates, typically 0.3 to 10+ microns, peak@3.5microns

Note that although their particulate size sensitivities overlap, their optimal particle size and concentration responsiveness is different between sensors. Thus, particle mass concentration and number are extrapolated based on the evaluation of sensor modality and empirical laboratory measurements.

PM Cartridge Layout

The PM Cartridge and its sensors are illustrated below:



The exhaust sample gas is drawn through the PM cartridge at ~1 liter per minute and first enters the Ionization Sensor.

Ionization Sensor

The sensor consists of a flow chamber, collector plate and a low-level alpha particle source (1 microcurie of Americium 241 foil) mounted on a grounded (negative) pedestal. The alpha particles are absorbed by the few centimeters of sample air/gas and the chamber enclosure to pose no safety risk. As the alpha particles collide with the sample gas air molecules they are split into positive and negative ions. The ion flow creates a measured continuous current flow between the positive plate and negative source.

As particulates enter the sensor chamber, the current flow is reduced by the disturbance of ion flow and provides a means to measure the magnitude of particulate matter.

Scattering Sensor

The scattering sensor measures the light from a 920 nm LED that is scattered toward a light receiver at 45° away from the incident forward direction. An electronic amplifier circuit is used to increase the sensitivity of the device to collaborate with the other sensors in the system. As the exhaust air sample flows through the chamber, the particulate scatter voltage signal is measured and recorded.

Opacity Sensor

The opacity sensor measures the amount of light attenuated by the particulates along a defined collimated light path length. Key components in the chamber tube include: (1) LED white light source; (2) a green light filter (to match standardized historical smoke meter preferences for green light); (3) light baffles along the light path to block stray uncollimated light and reflections from the interior walls of the tube; (4) sight glass at each end of the tube chamber to seal in the flowing sample gas and direct the light beam to the receiving light sensor; (5) photodiode (light receiver). When we combine the relative luminous intensity of white light, spectral percent transmission of the green filter, and the spectral responsivity of the photodiode, the final peak sensitivity is around 540 nm.

After passing through all sensors, the exhaust sample gases continue to flow out to a particulate filter, flow pump, and an exhaust outlet.

The voltage data measured from all sensors is continuously transmitted via Bluetooth to a laptop that records and calculates Particle Number and Mass based on standardized comparison reference data.

Key Take-Aways of the PM Cartridge

- Multi-plex approach using three dissimilar sensors to measure particulate matter.
- Calibration to Particle Number and Particle Mass via inversion of empirical laboratory data.
- Small sensors are contained within easily replaceable sensor cartridges.
- No dilution of the sample (No need to extrapolate the sensor values to full concentration).
- Physics of measurement are fundamentally identical to classic PEMS equipment.
- Comparable accuracy to larger, more expensive instrumentation.

Physics of the PM Sensors

Ionization

Ionization sensors are far more sensitive to ultra-fine particulates than opacity and scattering sensors. Ionization sensors have been an important part of emission analyses (see diffusion charging sensors).

If we assume that the particles in the air are of uniform size, then the diffusion motion of ions are shown to have a linear response to the particle surface area concentration detected in the sample. If not, then an approximation typically is be made over the range of particle sizes; typically, the models and experimental data show that particles' sizes would be in a log-normal distribution. For ease of use, virtually all ionization sensors have compensators to make their response linearly proportional to the particle size.

Specifically, the following system of equations govern the detector response:

$$\Delta I = I_1 - I_0$$
$$x = \Delta I / I_0$$
$$N_t = f_v / (18.62 * r_m^2)$$
$$Y = x * (2 - x) / (1 - x)$$
$$Y = k * N_t * r_m$$

Where,
I_0 = original current in the detector
I_1 = measured current in the detector
k = constant (determined empirically)
N_t = total number of particles passing through the chamber
r_m = mean particle radius
y = detector response

Opacity

Opacity, also known as extinction, is governed by the Beer-Lambert law as given below. Measuring obstruction and diffusion, the greater the number of particles per unit volume and/or the greater the average size of the particles, the higher the opacity.

$$\text{Opacity, } O = 1 - \exp(-n*a*q*l)$$

Where,
a = mean projected area (*or* attenuation cross-section *or* effective cross-sectional area)
l = path length of beam through the sample (technically, the length of effluent path)
n = number of particles per unit volume
q = particle extinction coefficient

The particle extinction coefficient varies versus wavelength and particle size. These numbers have been determined empirically at different wavelengths for different particles. The highest spectral responsivity of typical opacity sensors is in the green color wavelength range and the parSYNC achieves the same result by using a white LED and green filter. Opacity is measured by the change in the current within the circuit that the opacity meter resides. There are known limitations with using green light, such as the cross-sensitivity to NO_2. It is possible to use other color sources, however, each option has disadvantages. For example, red light is less sensitive to smaller particles and ultra-violet light is sensitive to methane.

The Beer-Lambert law applies over a wide range of concentrations and particles and, therefore, opacity sensors are useful to get an overall picture of the particle mass flow. However, opacity sensors are known to be less accurate when there is a lot of light scattering within the sample and when the particles are very small. To counter these issues, the parSYNC includes a scattering sensor (sensitive to larger particles and when large amounts of scattering occur) and an ionization sensor (sensitive to ultra-fine particles).

Scattering

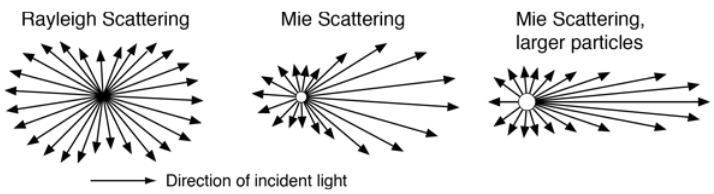
A greater number of particles will result in a greater amount of scattering; different sized particles along with greater number of particles will affect the scattering profile, which in turn varies by angle.

For non-absorbing particles, the following formula defines the scattering sensor's response to the incoming light for Rayleigh scattering:

$$I / I_0 = (\pi^4 / 8) * ((n^2 - 1) / (n^2 + 2))^2 * (D^6 / (r^2 * \lambda^4)) * (1 + \cos^2\theta)$$

Where,
n = index of refraction
D = particle diameter
r = distance of particle from light source
λ = wavelength of incident light
θ = scattering angle

Experimental data show that for comparatively uniform particle geometry and particle mass, the mass concentration versus scattering is log-linear in the Rayleigh region. Hence, the electronics within a scattering sensor can convert its readings to a usable output. It is well-known that the scattering sensors are most sensitive to larger particles, as can be inferred from the 6^{th} power on the particle diameter, D, factor in the above formula.



For large particles, we are in the geometric scattering region. The equation is modelled with an inhomogeneous wave equation with dissipation, as in:

$$u_{tt} - \Delta u - r^2 u = f(x, t)$$

with the appropriate initial and boundary conditions. This has known closed-form fundamental solutions of the form

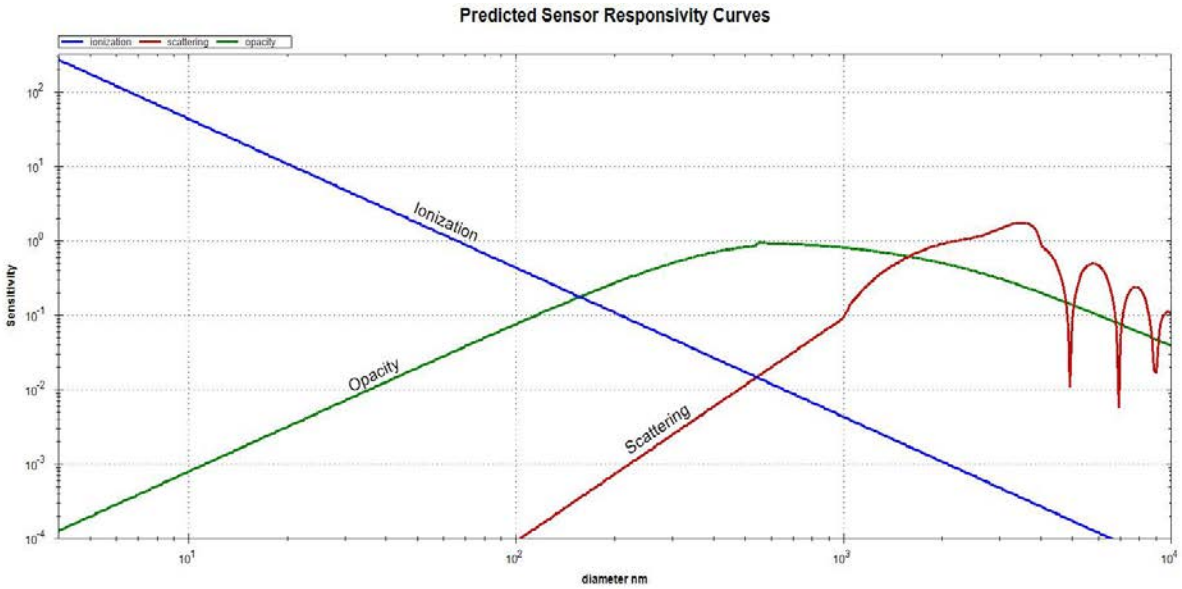
$$e^{kx} (A(x, t) \cos(\omega t) + C(x, t) \sin(\omega t))$$

where k is the spatial decay constant and ω is the frequency of the light source. This equation applies for large particles in the geometric scattering region.

(Note: Because of the dependencies on both angle and wavelength, varied incident angles and wavelengths can provide a more complete picture of the distribution.)

PM Sensor Response Curves

The relative sensitivity of each sensor, based on its theoretical response to particle diameter, is shown in the subsequent figure. The responses have been re-scaled to illustrate all sensors on the same graph. Wavelengths (and angles) of incident light used in the theoretical response calculations match the 3DATX sensors.



Note that each sensor type has a different peak sensitivity to particle size in identical situations. The Opacity sensor has a peak in the 0.8 micron diameter range (800 nm) and Scattering sensor peaks in the 3.5 micron diameter range. The parSYNC can perceive changes in the distribution of the size of the particles by using this physical property. These results have been quantified in laboratory tests.

Evaluating the response of the parSYNC sensors in a laboratory FTP-75 dynamometer test cycle yields measured response characteristics that closely follow the theoretical responsivity. For example, the test of a light-duty diesel vehicle with DPF yielded the data presented in the figure below. In this test, a TSI EEPS-3090 was used as a laboratory spectrometer reference. When characterizing the measured voltage response of the sensors to the ultra-fine particles, an illustrated log-linear graph below was determined from laboratory data measuring up to 520 nm diameter.