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Self-calibrated spectroscopic and AI-based gas analyzer

Abstract

Aspects relate to a compact and low-cost gas analyzer that can be used for different types of gas analysis, such as air quality analysis. The gas analyzer can include a light source, a gas cell configured to receive a sample (e.g., a gas under test), a spectral sensor including a spectrometer and a detector, and an artificial intelligence (AI) engine. Light can enter the gas cell and interact with the sample to produce output light that may be measured by the spectral sensor. The resulting spectrum produced by the spectral sensor may be analyzed by the AI engine to produce a result. The gas analyzer further includes a self-calibration component configured to enable calibration of the sample spectrum to compensate for spectral drift of the spectral sensor.

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Background/Summary

PRIORITY CLAIM (1) This application claims priority to and the benefit of Provisional Application No. 63/218,885, filed in the U.S. Patent and Trademark Office on Jul. 6, 2021, the entire content of which is incorporated herein by reference as if fully set forth below in its entirety and for all applicable purposes.

TECHNICAL FIELD
(1) The technology discussed below relates generally to spectroscopic-based gas analysis, and in particular to a spectroscopic artificial intelligence (AI)-based gas analyzer that is self-calibrated.
BACKGROUND
(2) Various technologies have been developed for gas sensing, including for example, technologies based on metal oxide semiconductor, polymer, carbon nanotubes, moisture absorption material, optical methods, calorimetric methods, gas chromatography and acoustic methods. Optical methods may be based on spectroscopy, interferometry, or ellipsometry, where the sensing occurs for the refractive index, absorbance and/or fluorescence properties of the analyte molecules or a chemo-optical transducing element. Multi-pass gas cells may be used in optical methods to increase the path length and improve the limit of detection. Examples of multi-pass gas cells include, but are

not limited to, White cells, Herriot cells, Pfund cells, and circular cells. Optical methods provide an advantage over other technologies with respect to sensitivity, response time, and the ability to detect a wide range of gases. However, optical methods can suffer from challenges related to the production cost of the optical sensor and the size of the volume optics components used in the analyzing system.

(3) To identify a gas sample under test (SUT) using optical methods, a background measurement (e.g., a background spectrum) is typically obtained and compared to a sample measurement (e.g., a sample spectrum) in order to abstract the specific gases absorptions from the sample measurement. The background measurement is usually performed before acquiring the spectrum of the sample. The background measurement does not contain any gases absorption, and as such, the background measurement can account for the transfer function of the measurement system, which may include, for example, a light source, a spectrometer, a detector and an optical coupling system. A challenge in obtaining background measurements involves evacuating the gas cell before each sample measurement to acquire the background spectrum, which may not be practical, for example, in examples in which the system is configured to obtain continuous measurements of gases flowing through the system.

(4) In one example, the background measurement of a reference gas cell may be obtained at the same time as a sample measurement of a different sample gas cell containing the sample under test. For example, the background measurement and sample measurement may be performed in parallel either using two separate spectrometers and detectors or using the same spectrometer and detector. As another example, the reference gas cell and the sample gas cell can be measured in series with a condition that the reference gas cell is filled with a non-interfering gas with the sample. However, this architecture requires the use of two different gas cells placed in parallel or in series with one another.

(5) In addition to the challenge of background measurements, the presence of mid-infrared (mid-IR) absorbing molecules in the atmosphere, such as water (H_2O) and carbon dioxide (CO_2), further presents a challenge of infrared (IR) spectroscopy in the open environment because the spectral contribution of atmospheric gases can hinder the accurate identification and quantification of target analytes. This problem is significant for water vapor as it has several strong absorption bands in the infrared region that overlap those of the target gases. There are two main challenges for the compensation of the absorption of water. The first challenge is that there is a non-linear relation between measured absorbance and true absorbance at low resolution and high absorbance. Therefore, the spectrum cannot simply be scaled by a factor with an assumption that this scaling factor accounts for the concentration change. The second challenge is that the water absorption spectrum is significantly dependent on environmental conditions, such as the temperature and pressure change.

SUMMARY

(6) The following presents a summary of one or more aspects of the present disclosure, in order to provide a basic understanding of such aspects. This summary is not an extensive overview of all contemplated features of the disclosure, and is intended neither to identify key or critical elements of all aspects of the disclosure nor to delineate the scope of any or all aspects of the disclosure. Its sole purpose is to present some concepts of one or more aspects of the disclosure in a form as a prelude to the more detailed description that is presented later.

(7) In an example, a self-calibrated and AI-based gas analyzer is disclosed. The gas analyzer includes a light source configured to produce incident light and a gas cell configured to receive a sample. The gas cell is further configured to receive input light corresponding to the incident light or an interference beam produced based on the incident light and to produce output light based on light interaction with the sample within the gas cell in a measurement mode. The gas analyzer further includes a spectral sensor including a spectrometer configured to receive the incident light from the light source or the output light from the gas cell and further configured to produce the

interference beam, where the interference beam corresponds to the input light or is produced based on the output light. The spectral sensor further includes a detector configured to obtain a sample spectrum of the sample based on the interference beam. The gas analyzer further includes an artificial intelligence engine configured to receive the sample spectrum and to generate a result indicative of at least one parameter associated with the sample based on the sample spectrum, control circuitry configured to control the light source and the spectral sensor, and a self-calibration component configured to enable calibration of the sample spectrum to compensate for spectral drift of the spectral sensor.

(8) These and other aspects of the invention will become more fully understood upon a review of the detailed description, which follows. Other aspects, features, and embodiments of the present invention will become apparent to those of ordinary skill in the art, upon reviewing the following description of specific, exemplary embodiments of the present invention in conjunction with the accompanying figures. While features of the present invention may be discussed relative to certain embodiments and figures below, all embodiments of the present invention can include one or more of the advantageous features discussed herein. In other words, while one or more embodiments may be discussed as having certain advantageous features, one or more of such features may also be used in accordance with the various embodiments of the invention discussed herein. In similar fashion, while exemplary embodiments may be discussed below as device, system, or method embodiments it should be understood that such exemplary embodiments can be implemented in various devices, systems, and methods.

Description

BRIEF DESCRIPTION OF THE DRAWINGS
(1) FIG. **1** is a diagram illustrating a spectrometer according to some aspects.
(2) FIG. **2** illustrates an example of a workflow for building an AI engine according to some aspects.
(3) FIG. **3** is a diagram illustrating an example of a gas analyzer according to some aspects.
(4) FIG. **4** is a diagram illustrating another example of a gas analyzer according to some aspects.
(5) FIGS. **5**A-**5**C are diagrams illustrating another example of a gas analyzer according to some aspects.
(6) FIGS. **6**A-**6**C are diagrams illustrating examples of gas analyzer configurations according to some aspects.
(7) FIG. **7** is a diagram illustrating another gas analyzer configuration according to some aspects.
(8) FIG. **8** is a diagram illustrating another gas analyzer configuration according to some aspects.
(9) FIGS. **9**A and **9**B are diagrams illustrating another gas analyzer configuration according to some aspects.
(10) FIG. **10** is a diagram illustrating an example of a cloud-based configuration of gas analyzers according to some aspects.
(11) FIG. **11** is a diagram illustrating a gas analyzer including a thermal control unit according to some aspects.
(12) FIGS. **12**A-**12**D are diagrams illustrating example configurations of a thermal control unit of a gas analyzer according to some aspects.
(13) FIGS. **13**A and **13**B are diagrams illustrating spectra of an analyte (sample) under test using different apodization functions according to some aspects.
(14) FIGS. **14**A and **14**B are diagrams illustrating spectra of an analyte with water vapor using different apodization functions according to some aspects.
(15) FIGS. **15**A and **15**B are further diagrams illustrating spectra of an analyte with water vapor using different apodization functions according to some aspects.

(16) FIGS. **16**A and **16**B are diagrams illustrating examples of simulated spectra of an analyte with water vapor before and after atmospheric compensation according to some aspects.

(17) FIG. **17** is a diagram illustrating a spectra of an analyte with water vapor after compensation according to some aspects.

(18) FIGS. **18**A and **18**B are diagrams illustrating an example of a modified Herriot gas cell according to some aspects.

(19) FIG. **19** is a diagram illustrating an example of an asymmetrical Herriot gas cell according to some aspects.

(20) FIGS. **20**A and **20**B are diagrams illustrating an example of a modified Herriot gas cell including a self-calibration component according to some aspects.

(21) FIGS. **21**A and **21**B are diagrams illustrating an example of a White gas cell including a self-calibration component according to some aspects.

(22) FIG. **22** is a diagram illustrating an example of an insertion mechanism for inserting redirecting optical elements into a White gas cell according to some aspects.

(23) FIG. **23** is a diagram illustrating another example of an insertion mechanism for inserting redirecting optical elements into a White gas cell according to some aspects.

(24) FIGS. **24**A and **24**B illustrate an example of a circular gas cell including a self-calibration component according to some aspects.

(25) FIGS. **25**A and **25**B are diagrams illustrating an exemplary gas analyzer including a self-calibration component external to the gas cell according to some aspects.

(26) FIGS. **26**A and **26**B are diagrams illustrating another exemplary gas analyzer including a self-calibration component external to the gas cell according to some aspects.

(27) FIGS. **27**A and **27**B are diagrams illustrating another exemplary gas analyzer including a self-calibration component external to the gas cell according to some aspects.

(28) FIGS. **28**A and **28**B are diagrams illustrating other exemplary gas analyzer configurations including a self-calibration component external to the gas cell according to some aspects.

(29) FIGS. **29**A and **29**B are diagrams illustrating an exemplary gas analyzer including a self-calibration component within the gas cell according to some aspects.

(30) FIGS. **30**A and **30**B are diagrams illustrating other exemplary gas analyzer configurations including a self-calibration component external to the gas cell according to some aspects.

(31) FIG. **31** is a diagram illustrating another exemplary gas analyzer configuration including a self-calibration component external to the gas cell according to some aspects.

(32) FIGS. **32**A and **32**B are diagrams illustrating other exemplary gas analyzer configurations including a self-calibration component external to the gas cell according to some aspects.

(33) FIG. **33** is a diagram illustrating another exemplary gas analyzer configuration including a self-calibration component external to the gas cell according to some aspects.

(34) FIG. **34** illustrates an example of a gas analyzer including a self-calibration component external to a circular gas cell according to some aspects.

(35) FIG. **35** is a diagram illustrating an example of a gas analyzer enabling a real-time reference background measurement according to some aspects.

(36) FIG. **36** is a diagram illustrating an example of self-calibration by the AI engine according to some aspects.

(37) FIG. **37** is a diagram illustrating an example of a gas analyzer configuration for filtering the gas sample under test according to some aspects.

(38) FIG. **38** is a diagram illustrating an example of a gas analyzer including a self-calibration component providing self-correction according to some aspects.

(39) FIG. **39** is a diagram illustrating another example of a gas analyzer including a self-calibration component providing self-correction according to some aspects.

(40) FIG. **40** is a diagram illustrating an example of a gas analyzer including a self-calibration component providing self-referencing and self-correction according to some aspects.

(41) FIG. **41** is a diagram illustrating an example of spectra of volatile organic compounds.

DETAILED DESCRIPTION

(42) The detailed description set forth below in connection with the appended drawings is intended as a description of various configurations and is not intended to represent the only configurations in which the concepts described herein may be practiced. The detailed description includes specific details for the purpose of providing a thorough understanding of various concepts. However, it will be apparent to those skilled in the art that these concepts may be practiced without these specific details. In some instances, well known structures and components are shown in block diagram form in order to avoid obscuring such concepts.

(43) Various aspects of the disclosure relate to a compact and low-cost gas analyzer that can be used for different types of gas analysis, such as air quality analysis. The core of the gas analyzer is a spectroscopic device that is capable of obtaining a spectrum of light over a wideband for multi-material detection. For example, the gas analyzer can include a light source (e.g., a single broadband light source), a gas cell configured to receive a sample (e.g., a gas under test), a spectral sensor including a spectrometer and a detector (e.g., a single photodetector), and an artificial intelligence (AI) engine. In some examples, the gas cell can include an asymmetric Herriot gas cell in which the reflectors each have a different radius of curvature. Other types of gas cells, including White gas cells and circular gas cells may also be used.

(44) Light can enter the gas cell and interact with the sample to produce output light that may be measured by the spectral sensor. In one example, the incident light produced by the light source may enter the gas cell as input light and the output light from the gas cell may be input to the spectrometer to produce an interference beam that may be detected by the detector. In another example, the incident light produced by the light source may be directed towards the spectrometer and the resulting interference beam may be input to the gas cell as the input light. In this example, the output light from the gas cell may be directed to the detector. The resulting spectrum produced by the spectral sensor may be analyzed by the AI engine to produce a result. For example, the AI engine may deduce the quality of air and trigger or initiate an action based on the analysis results.

(45) The gas analyzer further includes a self-calibration component configured to enable calibration of the sample spectrum without using a reference gas cell to compensate for spectral drift of the spectral sensor without the need for a separate reference gas cell or evacuating the sample under test from the sample gas cell to obtain a background measurement. In some examples, the self-calibration component includes additional optical elements configured to redirect light through the gas cell without reflecting off the gas cell reflector(s) or to redirect light outside of the gas cell for input to the spectrometer. In other examples, the self-calibration component includes a moveable reflector within the gas cell that can be moveable between a first position at which a sample measurement is obtained and a second position at which a reference spectrum is obtained. In other examples, the self-calibration component may include a reflective material attached to a solenoid external to a circular gas cell, where the solenoid is configured to move the reflective material into and out of the light path of light directed into the circular gas cell to obtain a sample spectrum and a reference spectrum. In other examples, the self-calibration component is included within the AI engine. In still other examples, the self-calibration component may include a bandpass filter configured to be inserted at the output of the gas cell. In further examples, the self-calibration component can be included within the spectrometer.

(46) Using the gas analyzer device described herein, different aspects of air quality can be analyzed, including, for example, the concentration of volatile organic compounds (VOCs), or the detection, classification and quantification of odor types, among many different applications. The gas analyzer device further provides a modular approach in which additional sensors (e.g., physical or chemical sensors) assisting the spectral analyzer can be co-integrated in the analyzer. In addition, the gas analyzer device may further include an atmospheric compensation unit configured to reduce or eliminate the effect of the presence of undesired substances (e.g., H_2O or CO_2) in the

gas cell. For example, the atmospheric compensation unit may include filters for filtering the undesired substances before entering the gas cell. In other examples, the atmospheric compensation unit may be implemented within the AI engine or spectrometer, where different apodizations may be used. In still other examples, the atmospheric compensation unit may include one or more sensors to measure the undesired substance concentration, the temperature of the gas cell, and/or the pressure in the gas cell, so the substances can be deduced and subtracted from the measured spectrum using the AI engine based on a database.

(47) The gas analyzer can be operated in different manners, such as mounting the gas analyzer in locations in which natural air flow leads force the air to enter and exit the gas cell. In other examples, the gas cell may be working in an inline operation or the gas analyzer can be equipped with a pump for generating the air flow and controlling the pressure of the air in the system. The gas analyzer may further be mounted in one or more locations in a heating, ventilation, and air conditioning (HVAC) system to monitor the air quality in different portions of the system. In addition, the gas analyzer can be mounted in vehicles for monitoring the air inside the car or monitoring the outdoor air in the environment. A network of the gas analyzers, together with a cloud-based AI engine, could be used to provide mapping of gas concentrations, based on numerical modeling of gas dispersion and the assimilation of the collected measured data.

(48) FIG. **1** is a diagram illustrating a spectrometer **100** according to some aspects. The spectrometer **100** may be, for example, a Fourier Transform infrared (FTIR) spectrometer. In the example shown in FIG. **1**, the spectrometer **100** is a Michelson FTIR interferometer. In other examples, the spectrometer may include an FTIR Fabry-Perot interferometer.

(49) FTIR spectrometers measure a single-beam spectrum (power spectral density (PSD)), where the intensity of the single-beam spectrum is proportional to the power of the radiation reaching the detector. In order to measure the absorbance of a sample, the background spectrum (i.e., the single-beam spectrum in absence of a sample) may first be measured to compensate for the instrument transfer function. The single-beam spectrum of light transmitted or reflected from the sample may then be measured. The absorbance of the sample may be calculated from the transmittance, reflectance, or trans-reflectance of the sample. For example, the absorbance of the sample may be calculated as the ratio of the spectrum of transmitted light, reflected light, or trans-reflected light from the sample to the background spectrum.

(50) The interferometer **100** includes a fixed mirror **104**, a moveable mirror **106**, a beam splitter **110**, and a detector **112** (e.g., a photodetector). A light source **102** associated with the spectrometer **100** is configured to emit an input beam and to direct the input beam towards the beam splitter **110**. The light source **102** may include, for example, a laser source, one or more wideband thermal radiation sources, or a quantum source with an array of light emitting devices that cover the wavelength range of interest.

(51) The beam splitter **110** is configured to split the input beam into two beams. One beam is reflected off of the fixed mirror **104** back towards the beam splitter **110**, while the other beam is reflected off of the moveable mirror **106** back towards the beam splitter **110**. The moveable mirror **106** may be coupled to an actuator **108** to displace the movable mirror **106** to the desired position for reflection of the beam. An optical path length difference (OPD) is then created between the reflected beams that is substantially equal to twice the mirror **106** displacement. In some examples, the actuator **108** may include a micro-electro-mechanical systems (MEMS) actuator, a thermal actuator, or other type of actuator.

(52) The reflected beams interfere at the beam splitter **110** to produce an output light beam, allowing the temporal coherence of the light to be measured at each different Optical Path Difference (OPD) offered by the moveable mirror **106**. The signal corresponding to the output light beam may be detected and measured by the detector **112** at many discrete positions of the moveable mirror **106** to produce an interferogram. In some examples, the detector **112** may include a detector array or a single pixel detector. The interferogram data verses the OPD may then be input to a

processor (not shown, for simplicity). The spectrum may then be retrieved, for example, using a Fourier transform carried out by the processor.

(53) In some examples, the interferometer **100** may be implemented as a MEMS interferometer **100***a* (e.g., a MEMS chip). The MEMS chip **100***a* may then be attached to a printed circuit board (PCB) **116** that may include, for example, one or more processors, memory devices, buses, and/or other components. In some examples, the PCB **116** may include a spectrum analyzer, such as an AI engine, configured to receive and process the spectrum. As used herein, the term MEMS refers to the integration of mechanical elements, sensors, actuators and electronics on a common silicon substrate through microfabrication technology. For example, the microelectronics are typically fabricated using an integrated circuit (IC) process, while the micromechanical components are fabricated using compatible micromachining processes that selectively etch away parts of the silicon wafer or add new structural layers to form the mechanical and electromechanical components. One example of a MEMS element is a micro-optical component having a dielectric or metallized surface working in a reflection or refraction mode. Other examples of MEMS elements include actuators, detector grooves and fiber grooves.

(54) In the example shown in FIG. **1**, the MEMS interferometer **100***a* may include the fixed mirror **104**, moveable mirror **106**, beam splitter **110**, and MEMS actuator **108** for controlling the moveable mirror **106**. In addition, the MEMS interferometer **100***a* may include fibers **114** for directing the input beam towards the beam splitter **110** and the output beam from the beam splitter **110** towards the detector (e.g., detector **112**). In some examples, the MEMS interferometer **100***a* may be fabricated using a Deep Reactive Ion Etching (DRIE) process on a Silicon On Insulator (SOI) wafer in order to produce the micro-optical components and other MEMS elements that are able to process free-space optical beams propagating parallel to the SOI substrate. For example, the electro-mechanical designs may be printed on masks and the masks may be used to pattern the design over the silicon or SOI wafer by photolithography. The patterns may then be etched (e.g., by DRIE) using batch processes, and the resulting chips (e.g., MEMS chip **100***a*) may be diced and packaged (e.g., attached to the PCB **116**).

(55) For example, the beam splitter **110** may be a silicon/air interface beam splitter (e.g., a half-plane beam splitter) positioned at an angle (e.g., 45 degrees) from the input beam. The input beam may then be split into two beams L**1** and L**2**, where L**1** propagates in air towards the moveable mirror **106** and L**2** propagates in silicon towards the fixed mirror **104**. Here, L**1** originates from the partial reflection of the input beam from the half-plane beam splitter **110**, and thus has a reflection angle equal to the beam incidence angle. L**2** originates from the partial transmission of the input beam through the half-plane beam splitter **110** and propagates in silicon at an angle determined by Snell's Law. In some examples, the fixed and moveable mirrors **104** and **106** are metallic mirrors, where selective metallization (e.g., using a shadow mask during a metallization step) is used to protect the beam splitter **110**. In other examples, the mirrors **104** and **106** are vertical Bragg mirrors that can be realized using, for example, DRIE.

(56) In some examples, the MEMS actuator **108** may be an electrostatic actuator formed of a comb drive and spring. For example, by applying a voltage to the comb drive, a potential difference results across the actuator **108**, which induces a capacitance therein, causing a driving force to be generated as well as a restoring force from the spring, thereby causing a displacement of moveable mirror **106** to the desired position for reflection of the beam back towards the beam splitter **110**.

(57) The unique information from the vibrational absorption bands of a molecule is reflected in an infrared spectrum that may be produced, for example, by the spectrometer **100** shown in FIG. **1**. By applying spectral numerical processing and statistical analysis to a spectrum, the information in the spectrum may be identified or otherwise classified. The application of statistical methods to the analysis of experimental data is traditionally known as chemometrics, and more recently as artificial intelligence.

(58) FIG. **2** illustrates an example of a workflow **200** for building an AI engine according to some

aspects. To begin building the AI engine, a group or population of samples **202** is obtained for measurements by a spectrometer, such as the spectrometer **100** shown in FIG. **1**, to produce spectra **204**. At the same time, these samples **202** can also be measured by conventional methods and the values recorded as reference values **206**. These reference values **206** together with the spectra **204** form a samples database **208** that is used to teach the AI engine (e.g., machine learning) how to interpret the spectra and transform the spectra to certain values (e.g., results). For example, the samples database **208** may be used in the development of statistical regression models (e.g., calibration models) **210** that may then be applied to a spectrum of a sample to produce a result associated with the sample. Validation and outliers detection **212** of the test results may then be performed to refine the calibration model(s).

(59) Since the spectrum produced by infrared (IR) spectroscopy are instantaneous, unlike conventional analysis methods, there is no need to wait for certain transformations (e.g., chemical transformations) to occur within the sample. Different physical and chemical parameters of the sample can be analyzed with a single scan.

(60) FIG. **3** is a diagram illustrating an example of a gas analyzer **300** according to some aspects. The gas analyzer **300** includes a gas cell **302**, a light source **304**, a spectral sensor **306**, an artificial intelligence (AI) engine **312**, a self-calibration component **314**, and control circuitry **316**. The control circuitry **316** may include, for example, one or more processor(s). For example, the processor(s) may include a single processing device or a plurality of processing devices. Such a processing device may be a microprocessor, micro-controller, digital signal processor, microcomputer, central processing unit, field programmable gate array, programmable logic device, logic circuitry, analog circuitry, digital circuitry, and/or any device that manipulates signals (analog and/or digital) based on hard coding of the circuitry and/or operational instructions. The control circuitry **316** may further include a memory, which may be a single memory device, a plurality of memory devices, and/or embedded circuitry of the processor. Such a memory device may be a read-only memory, random access memory, volatile memory, non-volatile memory, static memory, dynamic memory, flash memory, cache memory, and/or any device that stores digital information, including instructions (e.g., code) that may be executed by the processor.

(61) The spectral sensor **306** includes a spectrometer **308** and a detector **310**. The spectrometer **308** may include, for example, a Michelson interferometer, a Fabry-Perot cavity, or one more of light filters diffraction gratings, spatial light modulators, or birefringent devices. In some examples, the spectrometer **308** includes a MEMS interference device, such as the MEMS FTIR based spectrometer, as shown in FIG. **1**. The MEMS interferometer enables generating a spectrum in millisecond time scale since the moving micromirror is driven by a MEMS actuator. The detector **310** may include, for example, a single photodetector. The light source(s) **304** may include, for example, a laser source or wideband source. In some examples, the light source(s) **304** may be infrared or near-infrared light source(s). In an example, the light source **304** may include a single broadband light source.

(62) The gas cell **302** may be configured to receive a sample (e.g., a gas under test) **305**, such as air. The gas cell **302** may include, for example, a White cell (e.g., including three reflectors, such as three mirrors), a Herriot cell (e.g., including two reflectors, such as two mirrors), a Pfund cell, or a circular cell. The Herriot cell may be simpler than the White cell in that the Herriot cell includes only two mirrors and is less susceptible to mechanical disturbance of the cell. However, the Herriot cell may not accept high numerical aperture beams, and larger sized mirrors may be used when long path lengths are needed.

(63) The light source(s) **304** can be configured to generate incident light **318**. In some examples, as shown in FIG. **3**, the incident light **318** from the light source **304** may be directed into the gas cell (e.g., via one or more optical coupling elements, not shown) as input light. The gas cell **302** is a multi-pass gas cell configured to produce output light **320** based on light interaction with the sample via multiple reflections of the light within the gas cell **302**. The output light **320** may then

be input to the spectrometer **308**, which is configured to produce an interference beam **322** based on the output light **320**. The interference beam **322** may be received by the detector **310**, which may be configured to obtain a spectrum **324** of the sample based on the interference beam **322**.

(64) In other examples (shown by the dotted lines in FIG. **3**), the incident light **318** from the light source **304** may first be input to the spectrometer **308**. In this example, an interference beam **328** produced by the spectrometer **308** may be directed to the gas cell **302** as the input light that interacts with the sample via multiple reflections of light within the gas cell **302** to produce output light **330**. The output light **330** may then be detected by the detector **310** to obtain the spectrum **324** of the sample. In this configuration, the detector **310** can be detachable and replaced for modularity. The wavelength range of the spectral sensor **306** can be changed by changing the detector **310**. In addition, different cooling options for the detector **310**, such as one, two, three or four stages of cooling can be selected and used.

(65) The spectrum **324** may be input to the AI engine **312** for analysis and processing. The AI engine **312** is configured to process the spectrum **324** to generate a result **326** indicative of at least one parameter associated with the sample based on the spectrum **324**. For example, the AI engine **312** may include one or more processors for processing the spectrum **324** and a memory configured to store one or more calibration models utilized by the processor in processing the spectrum. In some examples, the result **326** corresponds to an action that is triggered or initiated based on the analysis of the spectrum **324**. For example, the action may include sending an alert to a control center or operator, evacuating a building, turning off an HVAC unit, control access to a building or facility, allow a human subject to pass through a gate, or other suitable action. In some examples, the result **326** may correspond to different aspects of air quality: (1) the concentration of volatile organic compounds (VOCs); (2) detection, classification, and quantification of odor types and levels thereof; (3) olfactometric analysis; (4) detection of biomarkers; (5) detection of particulate matter; (6) CO_2 concentration, CO concentration, NOx concentration, water vapor concentration, or humidity, in addition to any other physical or chemical analytes.

(66) The self-calibration component **314** may be configured to enable calibration of the sample spectrum **324** to compensate for spectral drift of the spectral sensor **306** without the use of a reference gas cell. In some examples, the self-calibration component **314** may facilitate self-referencing by enabling a reference spectrum (e.g., a background measurement) to be obtained by the detector **310** and input to the AI engine **312**. In other examples, the self-calibration component **314** may be included within the AI engine **312**. In still other examples, the self-calibration component **314** may be included within the spectrometer **308**. In still other examples, the self-calibration component **314** may be configured to provide for self-correction of the spectrum **324** that may be used separate from or together with the self-referencing.

(67) In an example operation, the control circuitry **316** can be configured to control the spectrometer **308** and the light source(s) **304** to initiate a measurement of a sample. For example, the control circuitry **316** can control the light source(s) **304** to generate and direct the incident light **318** to the gas cell **302** (or to the spectrometer **308**). The control circuitry **316** can further be configured to control the spectrometer **308** and detector **310** to produce the interference beam and transmit the spectrum **324** to the AI engine **312**. For example, the control circuitry **316** may be configured to power on/off the light source **304** and spectral sensor **306** and to provide other control signals to the light source **304** and the spectral sensor **306**. In addition, the control circuitry **316** may be configured to control the AI engine **312** to perform a particular analysis and/or to produce a particular result (e.g., turn on or off an HVAC unit, etc.). The control circuitry **316** may further be configured to control the self-calibration component **314**. For example, the control circuitry **316** may control the self-calibration component **314** to switch between a measurement mode in which the spectrum **324** of the sample within the gas cell is obtained and a calibration mode in which a reference spectrum (without the sample) is obtained.

(68) FIG. **4** is a diagram illustrating another example of a gas analyzer **400** according to some

aspects. The gas analyzer **400** shown in FIG. **4** includes a gas cell **402**, a light source **404**, a spectral sensor **406**, an artificial intelligence (AI) engine **412**, a self-calibration component **414**, and control circuitry **416**. As in the example shown in FIG. **3**, the light source(s) **404** can be configured to generate incident light **418**. In some examples, as shown in FIG. **4**, the incident light **418** from the light source **404** may be directed into the gas cell **402** (e.g., via one or more optical coupling elements, not shown) as input light, which interacts with the sample **405** within the gas cell **402** to produce output light **420**. The output light **420** may then be input to the spectrometer **408**, which is configured to produce an interference beam **422** based on the output light **420**. The interference beam **422** may be received by the detector **410**, which may be configured to obtain a spectrum **424** of the sample based on the interference beam **422**. The spectrum **424** may be input to the AI engine **412** for analysis and processing. The AI engine **412** is configured to process the spectrum **424** to generate a result **426** indicative of at least one parameter associated with the sample based on the spectrum **424**.

(69) In other examples (shown by the dotted lines in FIG. **4**), the incident light **418** from the light source **404** may first be input to the spectrometer **408**. In this example, an interference beam **428** produced by the spectrometer **408** may be directed to the gas cell **402** as the input light that interacts with the sample via multiple reflections of light within the gas cell **402** to produce output light **430**. The output light **430** may then be detected by the detector **410** to obtain the spectrum **424** of the sample.

(70) In the example shown in FIG. **4**, the gas analyzer **400** may further include a thermal control unit **432** configured to stabilize a temperature at the detector **410**. For example, the thermal control unit **432** may include a thermoelectric cooler (TEC), such as a Peltier element, heat sink(s), and/or fans. In addition, the gas analyzer **400** may further include a sample interface **434** configured to input the sample **405** into the gas cell **402**. For example, the sample interface **434** may provide an input to the gas cell **402** from a sampling environment **436**. Examples of sampling environments **436** include, but are not limited to, a monitoring area **438**, an HVAC system **440**, or a patient's breath **442** (e.g., exhaled air from a subject under test). In examples in which the sampling environment **436** corresponds to the breath of a patient **443**, the sample interface **434** may include, for example, disposable breath sampler (e.g., a mouthpiece or tube). In examples in which the sampling environment **436** corresponds to a monitoring area **436**, the gas analyzer **400** can be integrated, via the sample interface **434**, into vehicles, buildings, rooms, factories, storage areas, or any other indoor environment, or can be mounted, via the sample interface **434**, in an outdoor environment, such as oil and gas sites (e.g., for leakage monitoring and localization), leachate sites, and uncovered water sites.

(71) As in FIG. **3**, the control circuitry **416** is also configured to control the light source **404**, spectral sensor **406**, AI engine **412**, and self-calibration component **414**. For example, the control circuitry **416**, such as a microprocessor, can control the operation of the different components of the gas analyzer **400** and synchronize the operation of the light source **404**, the spectral sensor **406**, the thermal control unit **432**, and the self-calibration component **414**. In some examples, the gas analyzer **400** can be operating in different measurement modes. For example, the control circuitry **416** can switch on different components based on user input or to make a measurement at specified frequent discrete measurements. In case of continuous monitoring, the control circuitry **416** may continuously operate the gas analyzer components within specified active hours, collecting spectra continuously with a specified scan time/integration time. The control circuitry **416** can further continuously switch on/off various gas analyzer components, taking a measurement each specified period of time with a certain duty cycle to reduce the self-heating of the system or to improve the lifetime of the components, such that some components are switched off during the processing and the communication time.

(72) In addition, the gas analyzer **400** may further include one or more sensors **444** (e.g., physical or chemical or both types of sensors) that may also optionally be controlled by the control circuitry

416. Each of the one or more sensors **444** may be configured to generate sensor data related to the sample and to provide the sample data to the AI engine **412**. In some examples, the one or more other sensors **444** may include, for example, temperature, pressure, and/or flow sensors at the input and/or output of the gas cell **402** to record the flow of the air, temperature, and/or the pressure inside the gas cell **402**. Temperature, pressure and/or air flow sensors **444** can be used to enhance the accuracy of the prediction outputs of the AI engine **412**. For example, the temperature and pressure affects the molecular vibration spectrum of the gases, and the temperature may have a significant effect on hydrogen bonds, for example. The flow rate and pressure can also affect the equivalent concentration of the air constitutes in the gas cell **402**. In examples in which the gas analyzer is utilized in an HVAC system (HVAC environment **440**), flow rate sensor data may indicate the flow rate of the HVAC system (e.g., since HVAC systems can typically be operated at different flow rates). Other types of physical sensors **444** can be used for particulate matter, since such particulate matter affects light scattering that can lead to a baseline shift in the spectrometer **408** output.

(73) Chemical sensors **444** for some types of gases can also be integrated with the gas analyzer **400**. For example, some gases, such as O_2, H_2 and N_2, have almost no absorption in the infrared region of the spectrum since their vibrations are not accompanied with a change in the diploe moment. Therefore, detection of these types of gases can be performed using their electronic transition spectrum that is usually in the UV-V range. In this example, a UV-V spectral sensor **444** can be integrated in the gas analyzer **400**. Other types of gas sensors, such as electrochemical or another suitable type of gas sensor can also be used.

(74) The gas analyzer device **400** further includes an atmospheric compensation unit **446** configured to reduce an effect of the presence of one or more undesired substances in the gas cell **402**. In some examples, the atmospheric compensation unit **446** may be controlled by the control circuitry **416** and/or an output of the atmospheric compensation unit **446** may be provided to the AI engine **412**. In some examples, the undesired substances include CO_2 and/or water vapor (H_2O). Since the air contains a percentage of CO_2 and water vapor that are not negligible, especially for exhaled air from breath, and since both CO_2 and water vapor have strong infrared absorption signals, they may affect the prediction accuracy for other analytes in the air. Therefore, in some examples, the atmospheric compensation unit **446** includes additional sensors that may be used to quantify their presence, and the sensor output together with the spectrometer output may be fed into the AI engine **412** for improving the prediction accuracy of other analytes. For example, a humidity sensor can be used to correct for water vapor presence. In other examples, the atmospheric compensation unit **446** may be included within the AI engine **412** and/or the spectrometer **408** (e.g., the spectral sensor **406**).

(75) In some examples, the AI engine **412** may be implemented as or include a cloud-based AI engine **448**. In this example, data from the gas analyzer **400** (e.g., spectral data and sensor data) may be transmitted via a wireless or wireline connection to a cloud-based AI engine **446**. The cloud-based AI engine **446** may collect data from multiple gas analyzers to produce the result **426**. For example, a network of gas analyzers together with a modeling block in the cloud-based AI engine **446** may be used to provide mapping of gas concentrations, based on numerical modeling of gas dispersion and the assimilation of the collected measured data. In an example, for outdoor air monitoring, the gas analyzer **400** can be mounted in an outdoor environment, and data about the air quality can be continuously collected and communicated to the cloud-based AI engine **446** for air quality analysis. In another example, gas analyzers **400** can be mounted on vehicles and the data collected by the gas analyzers (and other sensors) may be wirelessly communicated to the cloud-based AI engine **446** to draw maps of pollution in cities based on the vehicle's mobility.

(76) The gas analyzer **400** is able to predict both chemical and physical parameters. For example, carbon dioxide, water vapor, total volatile organic compounds (TVOCs) are chemical parameters, while the particulate matter is a physical parameter. Part of the collected data may be used for

training the AI engine **412** using, for example, reference values from a reference device.

(77) FIGS. **5A**-**5C** are diagrams illustrating another example of a gas analyzer **500** according to some aspects. The gas analyzer **500** includes a gas cell **502**, a spectral sensor **504**, a light source **506**, control circuitry **508**, and optical coupling elements **510** (e.g., reflectors, such as mirrors). The gas cell **502** is a Herriot gas cell including two reflectors (e.g., two mirrors) **512** and **514**. In the example shown in FIG. **5A**, light from the light source **506** is optically coupled into the gas cell **502** using an input optical coupling element **510**. The light source **506** may be in the form of coherent light source, such as supercontinuum source or frequency comb, or in the form of uncoherent light source, such as thermal radiator or light emitting diode, plasma, or other suitable light source. The light interacts with the gas (air) under test within the gas cell **502** based on multiple reflections of the light therein, and the resulting output light is directed into the spectral sensor **504** via, for example, an output optical coupling element **510**. The spectral sensor **504** includes, for example, a spectrometer configured to produce an interference beam based on the output light. The interference beam is then optically coupled to a detector (e.g., photodetector) within the spectral sensor for the detection of light (e.g., detection of the interference beam) and energy conversion into an electrical form to produce a spectrum. The control module (e.g., a mother board) is used to power the light source **506** and power the spectral sensor **504**. In some examples, the optical coupling elements **510** may be optical lenses or reflectors.

(78) As shown in FIG. **5B**, gas (e.g., air) may be input to the gas cell **502** via a gas inlet **516** and exit the gas cell **502** via a gas outlet **518**. In some examples, as further shown in FIG. **5C**, the gas inlet and gas outlet may be coupled to a tube **520** (e.g., a sample interface) configured to provide the flow of gas into and out of the gas cell **502**. In addition, a valve **522** may be used to control the flow of the air/gas from an input **524** to an output **526**.

(79) FIGS. **6A**-**6C** are diagrams illustrating examples of gas analyzer configurations according to some aspects. In the example shown in FIG. **6A**, the gas analyzer main blocks include the gas cell **602** for light/air interaction and the spectroscopic unit (e.g., at least the light source and spectral sensor) **604** for analyzing the light. In some examples, the gas cell **602** may be considered to be a part of the spectroscopic unit **604**. The gas analyzer can be mounted such that the natural air flow leads **606** force the air to enter and exit the gas cell **602**.

(80) In another example, as shown in FIG. **6B**, the gas analyzer can be configured in an inline operation. For example, the gas analyzer can be inserted in air ducts **612** for ducted operation, such that the air flowing through the duct **612** enters the gas cell **608** for light/air interaction and the resulting output light may be measured by the spectroscopic unit **610**. In a further example, as shown in FIG. **6C**, the gas analyzer can be equipped with a pump **620** for generating the air flow and controlling the pressure of the air in the gas cell **614**. Filters (e.g., filter **618**) can be used as well to prevent dust particles or humidity condensation accumulating in the gas cell **614** or spectroscopic unit **616**. In this example, the gas analyzer can be mounted under a seat, above a roof, or localized in a corner. In each of the configurations shown in FIGS. **6A**-**6C**, the gas analyzer can be equipped with wireless communication capabilities for data transfer and/or powering.

(81) FIG. **7** is a diagram illustrating another gas analyzer configuration according to some aspects. For ducted operation, as shown in FIG. **7**, a tube connection **706** (e.g., sample interface) is used to interface the spectroscopic unit **702** and gas cell **704** within the spectroscopic unit **702** with the indoor/outdoor environment. One or more valves **708** may be used to control the flow of the air/gas from an input **710** to an output **712**. Other sensors, such as flow meters and pressure meters, can be used as well at the input **710** and/or output **712** to record the flow of the air and the pressure inside the gas cell. In some examples, the gas analyzer can be mounted in close proximity to oil and gas sites or gas pipes for leakage monitoring and localization.

(82) FIG. **8** is a diagram illustrating another gas analyzer configuration according to some aspects. In the example shown in FIG. **8**, a gas analyzer **802** can be mounted in one or more locations in an HVAC system **800**. For example, the gas analyzer **802** can be mounted on an output **808** of the

HVAC system **800** to monitor the supplied air from the HVAC system **800**. As another example, the gas analyzer **802** can also be mounted on a return air input **806** to the HVAC system **800** for monitoring the quality of the returned air. In both of the above examples, the indoor air quality is monitored. In a further example, the gas analyzer **802** can be mounted on an outdoor air input port **804** of the HVAC system **800** to monitor the quality of the outdoor air input to the system.

(83) FIGS. **9**A and **9**B are diagrams illustrating another gas analyzer configuration according to some aspects. In the example shown in FIG. **9**A, the gas analyzer **902** can be mounted in a vehicle **900** for monitoring the air inside the car (e.g., within an HVAC system **904**) or monitoring outdoor air in the environment **906**. In addition, the gas analyzer may be mounted under the seat or in the top of the car (not shown) to monitor the air quality inside the car (e.g., within the cabin). In examples in which the gas analyzer **902** is mounted in the HVAC system **904** of the car **900**, as shown in FIG. **9**B, the gas analyzer **902** can be mounted in a main path **910** in which the air is flowing or within a branch **912** of the main path **910** created for air monitoring that does not affect the main path. For outdoor air monitoring **906**, the gas analyzer **902** can be mounted behind the grill in the front of the car **900** or in any other place. With outdoor air monitoring **906**, data related to the air quality can be continuously collected while the vehicle **900** is moving. The vehicle **900** may further include a wireless device **908** or the gas analyzer **902** may be configured with a wireless transceiver to communicate the collected spectral data and any other related sensor data to a cloud-based AI engine for analysis.

(84) FIG. **10** is a diagram illustrating an example of a cloud-based configuration of gas analyzers according to some aspects. In the example shown in FIG. **10**, a wireless communication network including a plurality of gas analyzers **1002***a*-**1002***c* distributed over an area is realized. The gas analyzers **1002***a*-**1002***c* may be mounted, for example, within vehicles **1000***a*-**1000***c* moving within the area. A gateway **1006** may be used to collect data **1004***a*-**1004***c* sent by the gas analyzers **1002***a*-**1002***c* deployed over the area and to redirect the collected data **1004***a*-**1004***c* to a cloud-based AI engine **1008**. In some examples, the data **1004***a*-**1004***c* may include spectral data obtained by the spectroscopic unit (e.g., light source, gas cell, and spectral sensor) of the gas analyzer. In addition, the data **1004***a*-**1004***c* may further include sensor data (e.g., sensor readings, such as air flow, pressure, temperature, etc.) obtained by one or more sensors of the gas analyzer. The AI engine **1008** can implement a machine learning (ML) model (e.g., a neural network) to process the received data **1004***a*-**1004***c* using a calibration model that may be stored, for example, on a database **1010**. For example, the database **1010** may store sets of calibration models (e.g., statistical regression models) and the AI engine **1008** may select one of the calibration models for processing the data **1004***a*-**1004***c*. The AI engine **1008** may then transmit a result **1012***a*-**1012***c* to the vehicles **1000***a*-**1000***c* and/or the gas analyzers **1002***a*-**1002***c* produced based on the data **1004***a*-**1004***c*. For example, the result **1012***a*-**1012***c* may include air quality parameters and/or a recommended action.

(85) In some examples, the network of gas analyzers **1002***a*-**1002***c*, together with the cloud-based AI engine **1008**, may be configured to provide a mapping of gas concentrations, based on numerical modeling of gas dispersion and the assimilation of the collected measured data **1004***a*-**1004***c*. Different forms of mapping can be produced depending on the use case. For example, inverse modeling can serve for localization of gas leakages, if any. As another example, the cloud-based AI engine **1008** may use the collected data **1004***a*-**1004***c* to draw maps of pollution in cities based on the vehicles **1000***a*-**1000***c* mobility. Data from additional sensors determining the air flow speed and directions can be used to predict the dispersion of the pollution.

(86) In some examples, the AI engine may be localized in each of the gas analyzers **1002***a*-**1002***c*, and the data **1004***a*-**1004***c* and/or the result **1012***a*-**1012***c* may be transmitted to a database (not shown) for their storage. For example, a database may be set up on a server. This database can centralize all information needed for further processing of the collected data. In addition to the spectral and sensor data, other data, such as the location of sensors, the dates of receipt of the measurement, etc., may be stored in the database. In some examples, a library allows access to the

data without having to know the structure of the database may be provided.

(87) FIG. **11** is a diagram illustrating a gas analyzer **1100** including a thermal control unit according to some aspects. The thermal control unit is configured to stabilize the gas analyzer **1100** by cooling the components that are thermally sensitive, such as a detector. In some examples, the thermal control unit can include a Thermoelectric Cooler (TEC) **1114** for stabilizing the temperature at the detector (e.g., photodetector) of the spectral sensor **1102** (e.g., Light Modulation and Detection Module (LMDM)). The TEC **1114** can be mounted below a sensor board **1108** to control the temperature of the LMDM **1102**. For efficient operation, the conduction resistance should be very low between the TEC **1114** and the LMDM **1102**. For example, a hole can be drilled in the sensor board **1108** below the LMDM **1102**. Moreover, a super conductive material **1104** with a thermal interface material can be included to enhance the conduction between the LMDM **1102** and the TEC **1114**. The thermal conduction can also be enhanced by adding thermal vias or by embedding copper coin in the sensor board **1108** (e.g., printed circuit board (PCB)).

(88) From the other side of the TEC **1114**, a heat sink **1116** and a cooling fan **1118** can be included in the gas analyzer **1100** in order to dissipate the heat generated from the TEC **1114**. An electronics heat sink **1112** may further be included to dissipate heat from control electronics **1106** on the PCB **1108**. Insulator material **1110** between the heat sink **1116** and the PCB **1108** can also be added to prevent the heat from returning back to the PCB **1108**.

(89) In some examples, the TEC **1114** can be implemented in an open loop configuration with no feedback of temperature to the driving circuitry; however, this may not be suitable for variations in ambient temperature and changes in the self-heating conditions of the gas analyzer **1100**. Therefore, a closed-loop control loop may be used to ensure high accurate stabilization of the temperature of the LMDM **1102**, including a temperature sensor and a control chip (e.g., control electronics) **1106**. The control chip **1106** can include, for example, a proportional-integral-derivative (PID) controller, a difference amplifier, a compensation amplifier/network and an H-bridge. The difference amplifier can compare the current temperature sensor voltage with a target set-point temperature voltage resulting in an error voltage. The compensation amplifier/network can amplify the error signal, compensate and stabilize the feedback loop, and drive the next power/output stage. The H-bridge can control the magnitude and direction of TEC current to control whether it should cool or heat the gas analyzer **1100**. In some examples, the temperature sensor can be a thermistor beside or inside the LMDM **1102**, or a temperature sensor inside the control electronics **1106** next to the LMDM **1102** on the PCB **1108**. The temperature drift can also be extracted from the LMDM **1102** itself or specifically from the photodetector through spectral features drift.

(90) FIGS. **12A-12D** are diagrams illustrating example configurations of a thermal control unit of a gas analyzer according to some aspects. In the examples shown in FIGS. **12**A and **12**B, the thermal control unit can include a Peltier element (e.g., TEC) **1206** directly attached to the backside of a sensor board (e.g., PCB) **1204**, relying on the thermal conductivity of the board internal layers. A spectral sensor (e.g., light modulation chip of LMDM) **1202** may thus be attached to the topside of the PCB **1204**. A heat sink **1208** and fan **1210** may further be included under the TEC **1206** in order to dissipate the heat generated from the TEC **1206**. A thermistor **1212** adjacent the light modulation chip **1202** may provide a temperature of the light modulation chip **1202** to a control chip **1214** (e.g., control circuitry) via an electrical connection **1216** therebetween for closed-loop control of the TEC **1206**. In the example shown in FIG. **12**B, thermal conductivity between the light modulation chip **1202** and the TEC **1206** can be improved having a backside exposed pad **1220** soldered onto a sensor pad on the sensor board **1204** in addition to having thermal conduction vias **1218** in the sensor board **1204**.

(91) In the example shown in FIGS. **12**C and **12**D, a Peltier element (e.g., TEC) **1224** with a hole **1228** can be attached to the topside of the light modulation chip **1202**, such that light **1230** is coupled to the light modulation chip **1202** through the hole. A heat sink **1222** with a hole (e.g., hole

1228 through the heat sink **1222** and Peltier element **1224**) can be attached as well to the topside of the Peltier element **1224**. In addition, a fan **1226** can be included on the topside of the sensor board **1204** (e.g., PCB) to cool the heat sink **1222** and Peltier element **1224**. The thermistor **1212** may further be included on the topside of the PCB **1204** adjacent to the light modulation chip **1202** to measure the temperature of the light modulation chip **1202**.

(92) As discussed above, since the air contains a percentage of CO_2 and water vapor and both CO_2 and water vapor have strong infrared absorption signals, these undesired substances may affect the prediction accuracy for other analytes in the air. For example, gas absorption inside the gas cell can affect the interferogram bursts shape and position. However, the impact of the sample on the spectral sensor interferogram can be compensated, especially the sharp bands of CO_2 and water vapor, as described below. In some examples, the gas analyzer further includes an atmospheric compensation unit (e.g., atmospheric compensation unit **446** shown in FIG. **4**) configured to reduce an effect of the presence of one or more undesired substances in the gas cell. In some examples, as discussed above, the atmospheric compensation unit may include one or more additional sensors to quantify the presence of the undesired substances and the output data from the one or more additional sensors, along with the spectral sensor output, may be fed to the AI engine for improving the prediction accuracy of other analytes. For example, humidity sensor can be used to correct for water vapor presence.

(93) In other examples, the atmospheric compensation unit (e.g., atmospheric compensation unit **446** shown in FIG. **4**) may include an apodization function in the spectrometer of the spectral sensor (e.g., spectrometer **408** of the spectral sensor **406** shown in FIG. **4**) that can be used to reduce the impact of the presence of CO_2 and water vapor. The apodization function can be applied on the interferogram produced by the spectrometer. In various aspects, the apodization function applied on the interferogram can be studied for spectra of water vapor and Toluene to show how the water vapor peak and side lobes are affected by the apodization. For example, Gaussian and Boxcar apodization functions can be compared for Toluene spectra with different water vapor levels.

(94) FIGS. **13**A and **13**B are diagrams illustrating spectra of an analyte (sample) under test using different apodization functions according to some aspects. FIG. **13**A illustrates the spectra of pure Toluene with concentrations of 350, 700 and 1000 ppb at a resolution of 80 cm.sup.−1 and path length of 20 m using the Boxcar apodization, while FIG. **13**B illustrates the same spectra using the Gaussian apodization. As can be seen in FIGS. **13**A and **13**B, the Toluene peak has better resolution when Boxcar apodization is applied, but the sidelobes disappear in the case of Gaussian apodization.

(95) FIGS. **14**A and **14**B are diagrams illustrating spectra of an analyte with water vapor using different apodization functions according to some aspects. FIG. **14**A illustrates the spectra of Toluene with concentrations of 350,700 and 1000 ppb with a water vapor concentration of 0.14% at a resolution of 80 cm.sup.−1 and path length of 20 m using the Boxcar apodization, while FIG. **14**B illustrates the same spectra using the Gaussian apodization. It should be noted that a water vapor concentration of 0.14% is low compared to the usual water vapor atmospheric level. At the Toluene absorption region, there is water vapor absorption as the baseline is shifted. This shift is due to actual water vapor absorbance and not sidelobes of the water vapor peak because this shift is still clear even when Gaussian apodization is used.

(96) FIGS. **15**A and **15**B are further diagrams illustrating spectra of an analyte with water vapor using different apodization functions according to some aspects. FIG. **15**A illustrates the spectra of Toluene with concentrations of 350, 700 and 1000 ppb with water vapor of concentration 3% at a resolution of 80 cm.sup.−1 and path length of 20 m using the Boxcar apodization, while FIG. **15**B illustrates the same spectra using the Gaussian apodization. It should be noted that a water vapor concentration of 3% is close to the usual atmospheric levels. The weak absorption of Toluene is insignificant compared to the strong water vapor absorption in both apodizations.

(97) Therefore, to be able to measure small concentrations of Toluene at atmospheric conditions, the atmospheric compensation unit (e.g., atmospheric compensation unit **446** shown in FIG. **4**) may further include a water vapor compensation technique applied on the measured spectra by the AI engine (e.g., AI engine **412** or cloud-based AI engine **446** shown in FIG. **4**) and the spectrometer (e.g., spectrometer **408** shown in FIG. **4**). For example, a database of water vapor and/or CO_2 absorption spectrum at different temperatures and pressures can be formed either from experimental measurements or theoretically from existing databases, such as Pacific Northwest National Laboratory (PNNL), High-Resolution Transmission Molecular Absorption Database (HITRAN), or other available existing databases. The theoretical/experimental spectra can then be processed by the AI engine using synthesized spectral sensor characteristics, such the spectral resolution, self-apodization, baseline artifacts, thermal drift with temperature, etc., to produce processed spectra. The processed spectra may be provided by the AI engine to the spectrometer for application to the interferogram produced by the spectrometer. One simple example is direct subtraction of the processed spectra from the measured spectra by the spectrometer.

(98) In various aspects, the water vapor compensation technique can first be applied to simulated spectra of Toluene with water vapor to test the performance of this technique to eliminate water vapor absorption. FIGS. **16**A and **16**B are diagrams illustrating examples of simulated spectra of an analyte with water vapor before and after atmospheric compensation according to some aspects. The simulated spectra used are for 350 and 1000 ppb Toluene with 4% water vapor at a resolution 66 cm.sup.−1 and pathlength of 20 m. FIG. **16**A illustrates the spectra before compensation where the Toluene 350 ppb and Toluene 1000 ppb are not differentiated from each other due to the strong absorption of water vapor compared to the absorption of Toluene. FIG. **16**B illustrates the spectra after applying the atmospheric compensation method described above compared with true Toluene (pure 350 and 1000 ppb) spectra. FIG. **16**B illustrates the similarity between the spectra after applying the atmospheric compensation method and the spectra of pure Toluene.

(99) The water vapor compensation method discussed above can then be applied to the measured spectra of Toluene that contains different concentrations of water vapor. FIG. **17** is a diagram illustrating a spectra of an analyte with water vapor after compensation according to some aspects. The water vapor compensation method was applied on Toluene with concentrations of 7, 11 and 55 ppm with a resolution 80 cm.sup.−1 and a path length of 20 m. FIG. **17** illustrates the spectrum of Toluene 7 ppm before and after applying the compensation technique. As can be seen in FIG. **17**, the absorption decreased after the water vapor compensation method because the water absorption was eliminated.

(100) In an example in which the gas analyzer is mounted in a moving vehicle, the gas cell should be mechanically stable to prevent any changes in the optical path length or coupling efficiency of the light as a result of shock and vibration in the moving vehicle. In some examples, the size of the cell may be reduced to be more compact and to minimize the optical tolerance (of angles and decentering).

(101) FIGS. **18**A and **18**B are diagrams illustrating an example of a modified Herriot cell according to some aspects. The modified Herriot cell is an asymmetrical Herriot cell **1800** that is more compact and can tolerate vibrations when mounted in, for example, a moving vehicle. The asymmetrical Herriot cell **1800** includes a first reflector **1802** (e.g., mirror M**1**) and a second reflector **1804** (e.g., mirror M**2**) opposite the first reflector and configured to produce multiple reflections of light therebetween. To decrease the total number of reflections, as shown in FIG. **18**A, an angle A of incidence/reflection off the second reflector (M**2**) **1804** may be decreased and an angle B of incidence/reflection off the first reflector (M**1**) **1802** may be increased. This may be achieved by decreasing a radius of curvature C**1** of M**1** **1802** and increasing a radius of the curvature C**2** of M**2** **1804** according to the cell or cavity length. FIG. **18**B illustrates the multiple reflection light pattern in both a normal Herriot cell and in the modified (asymmetrical) Herriot cell.

(102) FIG. **19** is a diagram illustrating an example of an asymmetrical Herriot cell according to some aspects. An exemplary design of the asymmetric Herriot cell **1900** and the corresponding ray tracing is shown in FIG. **19**. In the example shown in FIG. **19**, the Herriot cell **1900** includes two reflectors **1902** and **1904** configured to produce multiple reflections therebetween. Each of the reflectors **1902** and **1904** has a different radius of curvature configured to reduce the total number of reflections. Light may enter the asymmetrical Herriot cell **1900**, for example, after being collimated by an off-axis parabolic mirror **1906**. Multiple reflections of light may then occur between the two reflectors **1902** and **1904** (e.g., mirrors M**1** and M**2**). Output light may then exit the Herriot cell **1900** and be focused onto the spectrometer (not shown) by an off-axis parabolic mirror **1908**.

(103) In some examples, the Herriot gas cell may not be able to be evacuated frequently for practical reasons. Therefore, a background (e.g., reference) measurement in a frequent manner may not be possible, and thus time drift in the light source, detector or light modulation chip response, for example, due to aging, may cause non-accurate prediction by the AI engine. In some examples, this may be overcome using a self-calibration mechanism (e.g., corresponding to the self-calibration component **314/414** shown in FIGS. **3** and **4**) in which the air is measured twice. One time with a path length L_1 and a second time with a path length L_2. The measured spectra S_1 and S_2 will be in the form of:

$$S_1 = P_{LS}(\lambda, t) R_d(\lambda, t) V_i(\lambda, t) \eta_1(\lambda) e^{-\alpha_{air}(\lambda) L_1} \quad \text{(Equation 1)}$$

$$S_2 = P_{LS}(\lambda, t) R_d(\lambda, t) V_i(\lambda, t) \eta_2(\lambda) e^{-\alpha_{air}(\lambda) L_2} \quad \text{(Equation 2)}$$

where $P_{LS}(\lambda, t)$ is the light source spectrum versus wavelength λ at a given aging time t, $R_d(\lambda, t)$ is the detector responsivity, $V_i(\lambda, t)$ is the light modulation chip response, for example, interferometer visibility, η is the coupling efficiency of the optics and α_{air} is the absorption coefficient of the gases in the air. By dividing the two measurements, a ratio may be obtained as follows:

$$S_1 / S_2 = \eta_1 / \eta_2 e^{-\alpha_{air}(\lambda)(L_1 - L_2)} \quad \text{(Equation 3)}$$

In this example, the ratio may be independent of the aging time. The AI calibration (or chemometrics) model may be trained using this ratio, and the prediction (e.g., result) can also be based on this ratio. For optimal detection with small limit of detection (LOD), the path L_1 can be maximized while the path L_2 is minimized.

(104) FIGS. **20**A and **20**B are diagrams illustrating an example of a modified Herriot gas cell including a self-calibration component according to some aspects. The modified Herriot gas cell **2000** is an asymmetric Herriot gas cell that includes two reflectors (e.g., mirrors) **2002** and **2004** configured to produce multiple reflections therebetween. Each of the reflectors **2002** and **2004** has a different radius of curvature configured to reduce the total number of reflections. Input light is coupled into the asymmetric Herriot gas cell **2000** via an input optical coupling element (e.g., an input off-axis parabolic mirror) **2006** and output light exits the asymmetric Herriot gas cell and is redirected towards a spectrometer (not shown) via an output optical coupling element (e.g., an output off-axis parabolic mirror) **2008**.

(105) In the example shown in FIG. **20**A, the self-calibration component corresponds to redirecting optical elements (e.g., mirrors) **2010** and **2012** that may be inserted into a light path of the modified Herriot cell **2000** to produce a short optical path length L_2. For example, the redirecting optical elements **2010** and **2012** may be inserted into the Herriot cell **2000** using a mechanical or electro-mechanical mechanism. Thus, the redirecting optical elements **2010** and **2012** may be configured to operate in a calibration mode to receive input light from the input optical coupling element **2006** and to redirect the input light through the Herriot gas cell without reflecting the light off either of the reflectors **2002** and **2004**. The resulting output light may be directed towards the

spectral sensor (not shown) via the output optical coupling element **2008**, where a reference spectrum may be obtained.

(106) In the example shown in FIG. **20**B, the redirecting optical elements **2010** and **2012** may be removed from the light path of the asymmetric Herriot cell **2000** (e.g., via a mechanical or electro-mechanical mechanism) to produce a long optical path length L.sub.1 and to enable a sample spectrum of a sample under test to be obtained in a measurement mode of the Herriot cell/gas analyzer. For example, input light may enter the asymmetric Herriot cell **2000** via the input optical coupling element **2006**. Multiple reflections of light may then occur between the two reflectors **2002** and **2004** to allow the reflected light to interact with a sample (not shown). Output light may then exit the Herriot cell **2000** and be focused onto the spectral sensor by the output optical coupling element **2008**.

(107) By inserting the redirecting mirrors **2010** and **2102** into the modified Herriot cell **2000**, the light system is common between the two measurements, with two optical path lengths L.sub.1 and L.sub.2 except for the optics inserted, which can change the coupling efficiency. This change in coupling efficiency may be kept time-independent by ensuring accurate placement of the optics from one measurement to another. Slight tolerance or misalignment may leads to a slight change, but this slight change is either wavelength independent or varies slowly with the wavelength as a baseline shift that can be overcome in the pre-processing in the AI engine.

(108) In some examples, the secondary optical path (e.g., optical path length L.sub.2) produced by the insertable redirecting optical elements **2010** and **2012** shown in FIG. **20**A may be a temporary path used for background calibration. In some examples, the secondary optical path does not affect the main path power, alignment, or function. However, the received power at the detector should be within a sufficient level. The self-calibration component (e.g., redirecting optical elements **2010** and **2012**) shown in FIG. **20**A can be adapted for other gas cells with different path lengths that may be optimized per application depending on the requirements on the detection range and limit of detection.

(109) FIGS. **21**A and **21**B are diagrams illustrating an example of a White gas cell including a self-calibration component according to some aspects. The White gas cell includes three reflectors (e.g., mirrors) **2102**, **2104**, and **2106**, an input optical coupling element (e.g., an input off-axis parabolic mirror) **2108**, and an output optical coupling element (e.g., an output off-axis parabolic mirror) **2110**. Each of the reflectors **2102**, **2104**, and **2106** may be a spherical mirror. In addition, each of the reflectors **2102**, **2104**, and **2106** may have the same radius of curvature that is equal to the separation (distance) between a larger spherical mirror **2102** on one side of the White gas cell **2100** and two smaller spherical mirrors **2104** and **2106** on the other side of the White gas cell **2100**. For example, spherical mirror **2102** may have a length that is greater than the respective lengths of either of spherical mirrors **2104** and **2106**. In addition, spherical mirrors **2104** and **2106** may be tilted with respect to one another to provide a small angle between the mirrors **2104** and **2106** selected to maintain the light within the White gas cell **2100**.

(110) In the example shown in FIG. **21**A, the White gas cell **2100** provides a long optical path length L.sub.1 to enable a sample spectrum of a sample under test to be obtained in a measurement mode of the White gas cell/gas analyzer. For example, input light can be coupled into the White gas cell **2100** via the input optical coupling element **2108**. Multiple reflections of light may then occur between the longer reflector **2102** and each of shorter reflectors **2104** and **2106** making at least two passes up and down the multi-pass White gas cell **2100** to allow the reflected light to interact with a sample (not shown). Output light may then exit the White gas cell and is redirected towards a spectrometer (not shown) via an output optical coupling element (e.g., an output off-axis parabolic mirror) **2110**.

(111) In the example shown in FIG. **21**B, the self-calibration component may include redirecting optical elements (e.g., two small mirrors) **2112** and **2114** that may be inserted into a light path of the White gas cell **2100** to switch from the main optical path L.sub.1 to the secondary optical path

L.sub.2. In some examples, the inserted mirrors **2112** and **2114** can be of the same type and have the same coating material as the White cell reflectors **2102**, **2104**, and **2106**, so that any degradation in the reflection will be common in the main optical path L.sub.1 and the secondary optical path L.sub.2. The second optical path directs the input light from the input optical coupling element **2108** into a U-turn path through the White gas cell **2100** towards the output optical coupling element **2110**. Thus, the redirecting optical elements **2112** and **2114** may be configured to operate in a calibration mode to receive input light from the input optical coupling element **2108** and to redirect the input light through the White gas cell **2100** without reflecting the light off any of the reflectors **2102**, **2104**, and **2106** to enable a reference spectrum of a sample under test to be obtained. In some examples, the redirecting optical elements **2112** and **2114** can be flat mirrors with alignment angle drivers, curved mirrors with decentering drivers, or wedges with alignment angle drivers. Examples of curved mirrors include, but are not limited to, concave, convex, or toroidal mirrors. The inserted redirecting optical elements **2112** and **2114** should satisfy the alignment between the cell input light and the output cell light.

(112) FIG. **22** is a diagram illustrating an example of an insertion mechanism for inserting redirecting optical elements into a White gas cell according to some aspects. The White gas cell **2200** includes three reflectors (e.g., mirrors) **2202**, **2204**, and **2206**, an input optical coupling element (e.g., an input off-axis parabolic mirror) **2208**, and an output optical coupling element (e.g., an output off-axis parabolic mirror) **2210**. Input light from a light source **2212** may be input to the White gas cell **2200** via the input optical coupling element **2208** and output light from the White gas cell **2200** may be coupled towards a spectral sensor (or detector) **2214** via the output optical coupling element **2210**.

(113) Redirecting optical elements **2216** and **2218** corresponding to the self-calibration component are mounted on a holder **2220**. The holder **2220** may be coupled to a lead screw **2222** (e.g., through a nut). The lead screw **2222** may be coupled to a bearing mechanism **2224** on one side and to a stepper motor **2226** on the other side for insertion and removal of the redirecting optical elements **2216** and **2218** into and out of the light path of the White gas cell **2200**, as described above in connection with FIG. **21**.

(114) FIG. **23** is a diagram illustrating another example of an insertion mechanism for inserting redirecting optical elements into a White gas cell according to some aspects. The White gas cell **2300** includes three reflectors (e.g., mirrors) **2302**, **2304**, and **2306**, an input optical coupling element (e.g., an input off-axis parabolic mirror) **2308**, and an output optical coupling element (e.g., an output off-axis parabolic mirror) **2310**. Input light from a light source **2312** may be input to the White gas cell **2300** via the input optical coupling element **2308** and output light from the White gas cell **2300** may be coupled towards a spectral sensor (or detector) **2314** via the output optical coupling element **2310**.

(115) Redirecting optical elements **2316** and **2318** corresponding to the self-calibration component may be inserted and removed from the light path of the White gas cell **2200** using a rotational motion instead of a translation motion as shown in FIG. **22**. The rotation can be around a hinge **2320** located at the sides of the White gas cell large reflector **2302**. The insertion mechanism shown in FIG. **23** reduces the overall size of the gas analyzer (e.g., as compared to the insertion mechanism shown in FIG. **22**), and does not complicate the optical design, since the redirecting optical elements **2316** and **2318** are not blocking any part of the light when the redirecting optical elements **2316** and **2318** are not inserted into the light path.

(116) FIGS. **24**A and **24**B illustrate an example of a circular gas cell including a self-calibration component according to some aspects. As shown in FIG. **24**A, the circular gas cell **2400** includes a circular reflecting element **2402**, an input **2404** and an output **2406**. Input light from a light source **2408** may be provided to the input **2404** of the circular gas cell **2400** via an input optical coupling element **2410** (e.g., one or more lenses or mirrors, such as an off-axis parabolic mirror). In a measurement mode of the circular gas cell/gas analyzer, multiple reflections of the input light may

occur within the circular gas cell **2400** around the circular reflecting element **2402** to produce light interaction with a sample under test within the circular gas cell **2400**. Output light may be directed via the output **2406** to an output optical coupling element **2412**, which is configured to couple the output light to a spectral sensor (or detector) **2414** to obtain a sample spectrum of the sample.

(117) In some examples, the circular gas cell **2400**, in the simplest shape, can be considered as a portion of sphere. In this example, the total path and number of reflections can be changed by tilting the input light away from the center of the sphere or by decentering the input light away from the center of the sphere (e.g., by five degrees). Different numbers of reflections and path lengths may be obtained using these two different options. However, the light at the circular gas cell output may spread and the light energy may be decreased. Therefore, in some examples, small divergence light sources such as lasers, may be used. However, the filament sources power may be decreased dramatically if used in this type of circular cell **2400**. Thus, in the filament source example, an array of spherical or toroidal mirrors may be included as the output optical coupling element **2412** to prevent the spreading of the light at the output **2406** of the circular cell **2400**.

(118) As shown in FIG. **24**B, the self-calibration component can include a flat mirror **2416** that may be inserted into the light path of the circular gas cell **2400**. When inserted, the flat mirror **2416** is configured to operate in a calibration mode to receive the input light via the input optical coupling element **2410** and to redirect the input light through the circular gas cell **2400** without reflecting off the circular reflecting element **2402** towards the output optical coupling element **2412** to obtain a reference spectrum. In some examples, the center of the flat mirror **2416** passes through the circle center of the circular gas cell **2400**. In addition, the flat mirror **2416** may be, for example, 60 mm by 10 mm, with a tilt around the flat mirror **2416** being five degrees.

(119) FIGS. **25**A and **25**B are diagrams illustrating an exemplary gas analyzer including a self-calibration component external to the gas cell according to some aspects. The gas analyzer **2500** includes a gas cell **2502** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **2504** and **2506**, though other types of gas cells may be used), optical coupling elements **2508** and **2510**, a light source **2512**, and a spectral sensor **2514** (e.g., spectrometer and associated detector). In a measurement mode of the gas analyzer **2500**, as shown in FIG. **25**A, incident light **2516** produced by the light source **2512** may be coupled into the gas cell **2502** as input light via an input optical coupling element **2508** (e.g., an off-axis parabolic mirror). The input light **2516** may be reflected between the two reflectors **2504** and **2506** to cause light interaction with a sample (not shown) within the gas cell **2502**. Output light **2518** from the gas cell **2502** may be coupled to the spectral sensor **2514** via an output optical coupling element **2510** (e.g., an off-axis parabolic mirror) to obtain a sample spectrum of the sample.

(120) In the example shown in FIG. **25**B, the self-calibration component includes external reflectors **2520** and **2522** outside of the gas cell **2502** and configured to operate in a calibration mode to receive the incident light **2516** produced by the light source **2512** and to produce reference light **2524** reflected towards the spectral sensor **2514** to obtain a reference spectrum without the sample. In some examples, the external reflectors **2520** and **2522** are coupled to an actuator **2526** that may be controlled, for example, by a control/processor chipset (e.g., control circuitry **316/416** shown in FIGS. **3** and **4**). Thus, in the calibration mode, self-referencing of the gas analyzer **2500** can be achieved automatically without the need for manual intervention or the need to pump the sample under test from the gas cell **2500**. The external reflectors **2520** and **2522** outside of the gas cell **2502** can be moved in-plane in-between the main optical coupling elements **2508** and **2510** and the gas cell **2502** to operate in the calibration mode, and then can be moved automatically out-of-plane to operate in the measurement mode. The external reflectors **2520** and **2522** prevent the incident light **2516** from entering the gas cell **2500** and direct the incident light **2516** to be coupled directly to the spectral sensor **2514** for measuring the background reference spectrum.

(121) FIGS. **26**A and **26**B are diagrams illustrating another exemplary gas analyzer including a self-calibration component external to the gas cell according to some aspects. The gas analyzer

2600 includes a gas cell **2602** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **2604** and **2606**, though other types of gas cells may be used), optical coupling elements **2608** and **2610**, a light source **2612**, and a spectral sensor **2614** (e.g., spectrometer and associated detector). In a measurement mode of the gas analyzer **2600**, as shown in FIG. **26**A, incident light **2616** produced by the light source **2612** may be coupled into the gas cell **2602** as input light via an input optical coupling element **2608** (e.g., an off-axis parabolic mirror). The input light **2616** may be reflected between the two reflectors **2604** and **2606** to cause light interaction with a sample (not shown) within the gas cell **2602**. Output light **2618** from the gas cell **2602** may be coupled to the spectral sensor **2614** via an output optical coupling element **2610** (e.g., an off-axis parabolic mirror) to obtain a sample spectrum of the sample.

(122) The self-calibration component in the example shown in FIGS. **26**A and **26**B includes two external reflectors **2624** and **2626** and a reference cell **2620** including a reference reflector **2622**. The two external reflectors **2624** and **2426** are attached to the main reflectors (e.g., optical coupling elements **2608** and **2610**), such that the four reflectors **2608**, **2610**, **2624**, and **2626** are moveable together (e.g., via an actuator as in the example shown in FIGS. **25**A and **25**B). In the measurement mode, as shown in FIG. **26**A, the two main reflectors **2608** and **2610** are aligned with the light source **2612** to direct the incident light **2616** along a gas cell path. In a calibration mode, as shown in FIG. **26**B, the external reflectors **2624** and **2626** are aligned with the light source **2612** to direct the incident light **2616** along a reference cell path. For example, the incident light **2616** may be directed by a first external reflector **2624** into the reference gas cell **2620**. The reference gas cell **2620** may be configured to receive the incident light reflected from the first external reflector **2624** and to reflect the incident light **2616** towards the second external reflector **2626** to produce reference light **2628** for reflection by the second external reflector **2626** towards the spectral sensor **2614**. In some examples, the reference gas cell **2620** can be a vacuum sealed cell or a cell of a short length to minimize the absorption of any gases in the air inside the cell.

(123) FIGS. **27**A and **27**B are diagrams illustrating another exemplary gas analyzer including a self-calibration component external to the gas cell according to some aspects. The gas analyzer **2700** includes a gas cell **2702** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **2704** and **2706**, though other types of gas cells may be used), optical coupling elements **2708** and **2710**, a light source **2712**, and a spectral sensor **2714** (e.g., spectrometer and associated detector). In a measurement mode of the gas analyzer **2700**, as shown in FIG. **27**A, incident light **2716** produced by the light source **2712** may be coupled into the gas cell **2702** as input light via an input optical coupling element **2708** (e.g., an off-axis parabolic mirror). The input light **2716** may be reflected between the two reflectors **2704** and **2706** to cause light interaction with a sample (not shown) within the gas cell **2702**. Output light **2718** from the gas cell **2702** may be coupled to the spectral sensor **2714** via an output optical coupling element **2710** (e.g., an off-axis parabolic mirror) to obtain a sample spectrum of the sample.

(124) The self-calibration component in the example shown in FIGS. **27**A and **27**B includes an actuator **2720** coupled to the optical coupling elements **2708** and **2710** (e.g., main reflectors). In this example, the actuator **2720** may be configured to move the main reflectors **2708** and **2710** away from the gas cell light path during calibration mode. Thus, the incident light **2716** produced by the light source **2712** may be coupled directly into the spectral sensor **2714** without passing through the gas cell **2702** and without being redirected by the main reflectors **2708** and **2710** or any other reflector.

(125) FIGS. **28**A and **28**B are diagrams illustrating other exemplary gas analyzer configurations including a self-calibration component external to the gas cell according to some aspects. The gas analyzers **2800***a* and **2800***b* shown in FIGS. **28**A and **28**B each include a gas cell **2802** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **2804** and **2806**, though other types of gas cells may be used), optical coupling elements **2808** and **2810**, a light source **2812**, and a spectral sensor **2814** (e.g., spectrometer and associated detector). In a

measurement mode of the gas analyzer **2800***a*, as shown in FIG. **28**A, incident light **2816** produced by the light source **2812** may be coupled into the gas cell **2802** as input light via an input optical coupling element **2808** (e.g., an off-axis parabolic mirror). The input light **2816** may be reflected between the two reflectors **2804** and **2806** to cause light interaction with a sample (not shown) within the gas cell **2802**. Output light **2818** from the gas cell **2802** may be directed towards the spectral sensor **2814** via an output optical coupling element **2810** (e.g., an off-axis parabolic mirror) to obtain a sample spectrum of the sample.

(126) In the example shown in FIGS. **28**A and **28**B, the self-calibration component includes two external reflectors **2820** and **2822** outside of the gas cell **2802** and configured to operate in a calibration mode to receive the incident light **2816** produced by the light source **2812** and to produce reference light **2826** reflected towards the spectral sensor **2814** to obtain a reference spectrum without the sample. The self-calibration component further includes a shutter **2824** configured to switch between the calibration mode and the measurement mode. For example, the shutter **2824** can be configured to block the reference light path during the measurement mode by blocking the incident light **2816** from reaching the second external reflector **2822**.

(127) In the example shown in FIG. **28**A, a beam combiner **2828** may be used to couple light from both the reference light path and the sample path (through the gas cell **2802**) to the spectral sensor **2814**. During reference measurement in calibration mode, the shutter **2824** may block the sample path (e.g., by blocking the output light **2818** from reaching the combiner **2828**) to be able to measure the reference spectrum separately, or the shutter **2824** may allow both paths to be coupled to the spectral sensor **2814**, such that the summation of the two spectra is collected. To extract the reference spectrum, the sample spectrum may be subtracted from the sum. For example, the beam combiner **2828** may be configured to combine the output light **2818** and the reference light **2826** for input to the spectral sensor **2814** to produce a combined spectrum in the calibration mode. The spectral sensor **2814** may then be configured to extract the reference spectrum from the combined spectrum by subtracting the sample spectrum from the combined spectrum.

(128) In some examples, the beam combiner **2828** can be in the form of typical beam splitter with a selected splitting ratio to maximize the coupled power from the sample path. Another option shown in FIG. **28**B includes a transmission diffuser **2832**, where the two beams of the two paths are focused onto the transmission diffuser **2832**. For example, the output light **2818** from the sample light path (e.g., from the gas cell **2802**) may be directed towards the transmission diffuser **2832** via the main optical coupling element **2810**, while the reference light **2826** from the reference light path (e.g., from the second external reflector **2822**) may be directed towards the transmission diffuser **2832** via an additional reflector **2830**. The output transmitted beam from the transmission diffuser **2832** can be considered as a new Lambertian source combining/mixing the two beams (output light **2818** and reference light **2826**), which may be directed towards the spectral sensor **2814**.

(129) FIGS. **29**A and **29**B are diagrams illustrating an exemplary gas analyzer including a self-calibration component within the gas cell according to some aspects. The gas analyzer **2900** includes a gas cell **2902** including a reflector **2904**, an optical coupling element **2906**, a light source **2908**, and a spectral sensor **2910**. The reflector **2904** may be a moveable reflector. For example, the moveable reflector **2904** may be coupled to an actuator for switching between a measurement mode (e.g., as shown in FIG. **29**A) and a calibration mode (e.g., as shown in FIG. **29**B). Incident light **2912** from the light source **2908** may be coupled via the optical coupling element (e.g., fixed reflector) **2906** into the gas cell **2902**. The light may then be directed towards the moveable reflector **2904**, which further reflects the light back towards the fixed reflector **2906** to produce output light/reference light **2914** coupled into the spectral sensor **2910**.

(130) In the example shown in FIGS. **29**A and **29**B, self-referencing can be achieved by measuring the spectra of the gas cell **2902** at two different path lengths by moving the moveable reflector **2904** between a first position in the measurement mode and a second position in a calibration

mode. In the measurement mode, as shown in FIG. **29**A, the spectral sensor **2910** may receive the output light **2914** from the gas cell **2902** produced based on light interaction with a sample (not shown) within the gas cell **2902** to obtain a sample spectrum corresponding to a long path length (Path length **1**) inside the gas cell **2902**. In the calibration mode, as shown in FIG. **29**B, the spectral sensor **2910** may receive the reference light **2914** from the gas cell **2902** to obtain a reference spectrum corresponding to a short path length (Path length **2**) inside the gas cell **2902**.

(131) FIGS. **30**A and **30**B are diagrams illustrating other exemplary gas analyzer configurations including a self-calibration component external to the gas cell according to some aspects. The gas analyzers **3000***a* and **3000***b* shown in FIGS. **30**A and **30**B each include a gas cell **3002** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **3004** and **3006**, though other types of gas cells may be used), optical coupling elements **3008** and **3010**, a light source **3012**, and a spectral sensor **3014** (e.g., spectrometer and associated detector). In a measurement mode of the gas analyzer **3000**, as shown in FIG. **30**A, incident light **3016** produced by the light source **3012** may be coupled into the gas cell **3002** as input light via an input optical coupling element **3008** (e.g., an off-axis parabolic mirror). The input light **3016** may be reflected between the two reflectors **3004** and **3006** to cause light interaction with a sample (not shown) within the gas cell **3002**. Output light **3018** from the gas cell **3002** may be directed towards the spectral sensor **3014** via an output optical coupling element **3010** (e.g., an off-axis parabolic mirror) to obtain a sample spectrum of the sample.

(132) In the example shown in FIG. **30**A, the self-calibration component includes external reflectors **3020** and **3022** outside of the gas cell **3002** configured to operate in a calibration mode to receive the incident light **3016** produced by the light source **3012** and to produce reference light **3028** reflected towards the spectral sensor **3014** to obtain a reference spectrum without the sample. The self-calibration component further includes an electro-optic controlled element **3024** configured to switch between the calibration mode and the measurement mode. For example, the electro-optic controlled element **3024** can be configured to block the reference light path during the measurement mode by blocking the incident light **3016** from reaching the second external reflector **3022**. In some examples, the electro-optic controlled element **3024** may be an electro-optic controlled-transmittance window of special material or an electrically controlled polarizer.

(133) The gas analyzer **3000** further includes a beam combiner **3026** configured to couple light from both the reference light path and the sample path (through the gas cell **3002**) to the spectral sensor **3014**. During sample measurement in measurement mode, the electro-optic controlled element **3024** may block the reference path (e.g., by blocking the incident light **3016** from reaching the second external reflector **3022**) to be able to measure the sample spectrum. In calibration mode, the electro-optic controlled element **3024** may allow both paths to be coupled to the spectral sensor **3014**, such that the summation of the two spectra is collected. To extract the reference spectrum, the sample spectrum may be subtracted from the sum.

(134) In the example shown in FIG. **30**B, the self-calibration component includes an interferometer **3032**, which may include retro-reflectors **3034** and **3036** and a beam splitter **3038**. One of the retro-reflectors **3034** and **3036** may be a moveable mirror configured to produce an optical path length difference between the two arms (e.g., the two light paths) of the interferometer **3032**. The optical path length difference between the two arms (light paths) in the interferometer may be controlled to enable switching between the calibration mode and the measurement. For example, in measurement mode, the optical path length difference may be controlled to produce an output interference pattern (e.g., reference light **3040**) adjusted to near the interferogram null. In calibration mode, the optical path length may be controlled to produce the reference light **3040** for a background measurement. The reference light **3040** may be coupled to a transmission diffuser **3044** via a coupling mirror **3042**, where the reference light **3040** of the reference path and the output light **3018** of the sample path are focused onto the transmission diffuser **3044**. The output from the transmission diffuser **3044** may be directed towards the spectral sensor **3014**.

(135) FIG. **31** is a diagram illustrating another exemplary gas analyzer configuration including a self-calibration component external to the gas cell according to some aspects. The gas analyzer **3100** includes a gas cell **3102** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **3104** and **3106**, though other types of gas cells may be used), optical coupling elements **3108** and **3110**, a light source **3112**, and a spectral sensor **3114** (e.g., spectrometer and associated detector). In the measurement mode of the gas analyzer **3100**, incident light **3116** produced by the light source **3112** may be coupled into the gas cell **3102** as input light via an input optical coupling element **3108** (e.g., an off-axis parabolic mirror). The input light **3116** may be reflected between the two reflectors **3104** and **3106** to cause light interaction with a sample (not shown) within the gas cell **3102**. Output light **3118** from the gas cell **3102** may be directed towards the spectral sensor **3114** via an output optical coupling element **3110** (e.g., an off-axis parabolic mirror) to obtain a sample spectrum of the sample.

(136) The self-calibration component includes external reflectors **3120** and **3122** outside of the gas cell **3102** configured to operate in a calibration mode to receive the incident light **3116** produced by the light source **3112** and to produce reference light **3126** reflected towards the spectral sensor **3114** to obtain a reference spectrum without the sample. The self-calibration component further includes an optical bandpass filter **3124** coupled between the external reflectors **3120** and **3122** and configured to produce the reference light **3126** including reference bands for input to the spectral sensor **3114**. Thus, the bandpass filter **3124** is configured to pass certain bands from reference path to be detected and monitored for baseline drifts compensation. Another complementary bandstop filter **3128** can be added in the sample path to filter-out the bands passed by the bandpass filter **3124**. The filter bands passed by the bandpass filter **3124** may be selected to be away from the important bands of the sample under test. In the example shown in FIG. **31**, the reference light **3126** may be coupled to a transmission diffuser **3132** via a coupling mirror **3130**, where the reference light **3126** of the reference path and the output light **3118** of the sample path are focused onto the transmission diffuser **3132**. The output from the transmission diffuser **3142** may be directed towards the spectral sensor **3114**.

(137) FIGS. **32**A and **32**B are diagrams illustrating other exemplary gas analyzer configurations including a self-calibration component external to the gas cell according to some aspects. The gas analyzers **3200**a and **3200**b shown in FIGS. **32**A and **32**B each include a gas cell **3202** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **3204** and **3206**, though other types of gas cells may be used), an optical coupling element **3208**, a light source **3210**, and a spectral sensor **3212** (e.g., spectrometer and associated detector). The light source **3210** is a dual filament light source including two adjacent filaments electrically separated with two different voltage terminals and a common ground terminal. Each filament is coupled to one of the sample path and the reference path. The two filaments can be switched in the time-domain, synchronized with the spectral sensor operation.

(138) In the example shown in FIG. **32**A, in the measurement mode, incident light **3214** (e.g., first input light) produced by one of the filaments of the light source **3210** may be coupled into the gas cell **3202** as input light via an input optical coupling element **3208** (e.g., an off-axis parabolic mirror). The input light **3214** may be reflected between the two reflectors **3204** and **3206** to cause light interaction with a sample (not shown) within the gas cell **3202**. Output light **3216** from the gas cell **3202** may be directed towards the spectral sensor **3212** to obtain a sample spectrum of the sample.

(139) The self-calibration component includes two external reflectors **3218** and **3220** (e.g., off-axis parabolic mirrors) outside of the gas cell **3202** and configured to operate in a calibration mode to receive incident light **3222** (e.g., second input light) produced by the other filament of the light source **3210** and to produce reference light **3224** reflected towards the spectral sensor **3212** to obtain a reference spectrum without the sample. A first external reflector **3218** is attached to the main reflector **3208** and aligned to receive the second input light **3222**. A beam combiner **3226** may

be used to couple light from both the reference light path and the sample path (through the gas cell **3202**) to the spectral sensor **3212**. In examples in which the dual filament light source **3210** is configured to switch between the first input light **3214** and the second input light **3222**, the gas analyzer **3200** may be configured to separately operate in measurement mode and calibration mode to obtain separate sample spectra and reference spectra. In some examples, during calibration mode, the light source **3210** may be configured to simultaneously produce both the first input light **3214** via the first filament and the second input light **3222** via the second filament. In this example, both the sample and reference paths may be coupled to the spectral sensor **3212** via the combiner **3226**, such that the summation of the two spectra is collected. To extract the reference spectrum, the sample spectrum may be subtracted from the sum.

(140) In the example shown in FIG. **32**B, the two beams of the two paths (sample and reference) are focused onto a transmission diffuser **3232**. For example, the output light **3216** from the sample light path (e.g., from the gas cell **3202**) may be directed towards the transmission diffuser **3232** via an additional optical coupling element **3228**, while the reference light **3224** from the reference light path (e.g., from the external reflector **3220**) may be directed towards the transmission diffuser **3232** via an additional reflector (mirror) **3230**. The output transmitted beam (combining/mixing the output light **3216** and reference light **3224**) from the transmission diffuser **3232** can be focused on spectral sensor **3214** via a lens **3234**.

(141) FIG. **33** is a diagram illustrating another exemplary gas analyzer configuration including a self-calibration component external to the gas cell according to some aspects. The gas analyzer **3300** includes a gas cell **3302** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **3304** and **3306**, though other types of gas cells may be used), an optical coupling element **3308**, a light source **3310**, and a spectral sensor **3312** (e.g., spectrometer and associated detector). In the measurement mode of the gas analyzer **3300**, incident light **3314** produced by the light source **3310** may be coupled into the gas cell **3302** as input light via an input optical coupling element **3308** (e.g., an off-axis parabolic mirror). The input light **3314** may be reflected between the two reflectors **3304** and **3306** to cause light interaction with a sample (not shown) within the gas cell **3302**. Output light **3316** from the gas cell **3302** may be directed towards the spectral sensor **3312** to obtain a sample spectrum of the sample.

(142) The self-calibration component includes external reflectors **3318** and **3320** outside of the gas cell **3302** configured to operate in a calibration mode to receive the incident light **3314** produced by the light source **3310** and to produce reference light **3322** reflected towards the spectral sensor **3312** to obtain a reference spectrum without the sample. In the example shown in FIG. **33**, self-referencing of the gas analyzer **3300** is achieved using a Michelson interferometer **3324** with a two-level mirror M in one of its arms. The interferometer **3324** can be added before the spectral sensor **3312**. The two levels of the mirror M lead to two reflected half-beams of an optical path difference $2d_o$ corresponding to double the mirror step. The output of the interferometer **3326** is a modulated light beam in spectral domain, with a relatively slow cosine function corresponding to the mirror step size, while another very fast sine function exists due to the interference between the sample path and the reference path as follows:

$$P=P_s(1+\cos(2kd_o))+P_{ref}-2\sqrt{(P_s P_{ref})}\sin(k(L_{ref}-L_s-d_o)) \qquad \text{(Equation 4)}$$

where P_s is the sample path power, P_{ref} is the reference path coupled power to the output of the interferometer, L_{ref} is the reference path length, and L_s is the sample path length. Such fast variations are due to the very long optical path difference between the two paths, and as such, a high resolution spectrometer (e.g., of the spectral sensor **3212**) is needed to capture the difference. Given that, the interferogram signal of the spectral sensor **3212** may include a secondary burst at a spectral sensor interferometer moveable mirror distance d_o. The mirror step d_o may be adjusted to result in the secondary burst being outside the interferogram window corresponding to the target resolution. The reference spectrum can be extracted from the

secondary burst, and then the main burst signal can be corrected to extract the sample spectrum.

(143) The self-referencing example shown in FIG. **33** can be used for self-correction as well, where the secondary burst position with respect to the main burst position can be used as a reference optical path difference to correct for any wavenumber drifts that may be due to optical path difference drifts.

(144) FIG. **34** illustrates an example of a gas analyzer including a self-calibration component external to a circular gas cell according to some aspects. As shown in FIG. **34**, the gas analyzer **3400** includes a circular gas cell **3402**, a light source **3404**, and a spectral sensor **3406**. The circular gas cell **3402** may be, for example, a single input/output toroidal gas cell, where the input is collimated light and the output light may be directed towards the spectral sensor **3406** to obtain a sample spectrum. In the example shown in FIG. **34**, the self-calibration component may include a solenoid **3408** attached to a reflective material **3410** that enables the source/detector **3404/3406** to be internal reference corrected. In this example, the reflective material **3410** may further operate as a mirror for focusing the output light onto the spectral sensor **3406** during measurement mode to obtain a sample spectrum. In addition, the solenoid **3408** may be configured to move the reflective material **3410** into a light path of the incident light from the light source **3404** in a calibration mode to prevent the incident light from entering the toroidal gas cell **3202** and to couple the incident light to the spectral sensor **3406** to obtain a reference spectrum. Thus, the background measurement is acquired while the incident light is reflected directly from the reflective material **3410**, and the solenoid **3408** is configured to move the reflective material **3410** away in order to allow the incident light to enter the gas cell **3402** to measure the sample under test. In some examples, the solenoid **3408** may be more robust to shock vibrations than moving mechanical mirrors, and may also be less sensitive.

(145) FIG. **35** is a diagram illustrating an example of a gas analyzer enabling a real-time reference background measurement according to some aspects. The gas analyzer **3500** includes a spectroscopic unit **3502** (e.g., at least a light source, gas cell, and spectral sensor). The spectroscopic unit may be coupled to a valve **3504** configured to allow airflow from an airflow input **3508** to enter the spectroscopic unit **3502** for sample measurement. In addition, the valve **3504** is further configured to stop the airflow into the spectroscopic unit **3502**. A downstream pump **3506**, which may be located adjacent to or removed from the spectroscopic unit **3506** is configured to pump the air out of the spectroscopic unit **3502** towards an airflow output **3510**. By closing the valve **3504** while the pump **3506** is on, a pseudo vacuum may be created in the spectroscopic unit **3502**, thus enabling a background measurement (e.g., reference spectrum) to be obtained while no (or minimal) gas is present in the gas cell of the spectroscopic unit **3502**. This enables an online/real-time reference background measurement. The gas analyzer **3500** may further include a temperature sensor **3512** and a pressure sensor **3514** configured to measure the temperature and pressure of the spectroscopic unit **3502**. The temperature and pressure measurements (e.g., sensor data) may be fed into an AI engine (not shown) to enable offset correction based on the temperature and pressure values. In addition, pumping while partially closing the valve (or having a secondary valve) may change the pressure and increase the dynamic range of the measurement by decreasing the amount of gas in the spectroscopic unit **3502**.

(146) In some examples, as described above, the self-calibration component may be included in the AI engine (e.g., AI engine **312/412** shown in FIGS. **3** and **4**). For example, the AI engine may be configured to perform self-referencing by using a special treatment of the measured spectra. In one example, a reference wavelength among the whole span of the measured wavelengths where the absorbance is independent of the sample under test concentration may be determined. Based on the reference wavelength, information regarding external fluctuations (drift, aging, etc.) can be measured according to the absorbance change at the reference wavelength and the spectrum can be corrected accordingly.

(147) In another example, self-referencing may be performed by inserting a well-designed optical

filter with specific transmission values at the different wavelengths (t.sub.1 at λ.sub.1, t.sub.2 at λ.sub.2, t.sub.3 at λ.sub.3 and so on) when re-calibration is needed. Taking advantage of the well-known relation between the different transmission values (t.sub.1, t.sub.2, t.sub.3, etc. . . .), the AI engine may correct the spectrum accordingly by removing the effect of any drift or aging with time of the different optical components in the system. In addition, this filter may be measured continuously without removal if it is designed with maximum transmission values at the wavelengths of interest where the sample absorption peaks exist to avoid any interference or loss in the signal to noise ratio. Light source drifts can be also compensated using dedicated photodetector(s) to monitor optical power drift of the light source within the band of interest or outside the band of interest.

(148) FIG. **36** is a diagram illustrating an example of self-calibration by the AI engine according to some aspects. To avoid measuring the background when it is not suitable for practical reasons, the background may be estimated using the AI engine by estimating the baseline for each sample measurement separately while considering it as the background and then subtracting the baseline to extract the superimposed peaks, which are the peaks of interest associated with the sample under test as shown by the sample measurement in FIG. **36**.

(149) In some examples, the gas sample under test may be pre-concentrated before introducing the sample into the gas cell. Pre-concentration of the sample may increase the capability of having a low limit of detection (LOD) and being able to measure very low concentrations of gases, such as in the case of measuring volatile organic compounds (VOCs). Different sorbent materials, such as Tenax, Carboxen, and other suitable materials may be used based on the gas under test in which the gas molecules are adsorbed by the sorbent materials. In this example, the gases may be released when the sorbent material is heated, leading to have a high concentration of the gas under test.

(150) In other examples, the input gas sample to the gas cell may be filtered to remove specific gases (e.g., H_2O, CO_2, etc.) that could mask the peaks of the sample under test. FIG. **37** is a diagram illustrating an example of a gas analyzer configuration for filtering the gas sample under test according to some aspects. In the example shown in FIG. **37**, the gas analyzer **3700** includes a spectroscopic unit **3702** (e.g., light source, spectral sensor, and gas cell). Gas (e.g., air) may be input to the spectroscopic unit **3702** via a gas inlet **3704** and exit the spectroscopic unit **3702** via a gas outlet **3706**. The gas inlet and gas outlet may be coupled to a tube **3708** (e.g., a sample interface) configured to provide the flow of gas into and out of the spectroscopic unit **3702**. In addition, a gas filter **3710** may be coupled between the tube **3708** and the gas inlet **3704** to filter the gas entering the spectroscopic unit **3702** (e.g., to remove specific gases from the gas sample under test).

(151) In some examples, a wavenumber/wavelength (x-axis) drift may occur with aging or when environmental conditions change. To automatically compensate for wavelength shifts, various aspects provide different self-correction (e.g., self-calibration) techniques. In one technique, self-correction can be achieved by monitoring the position of CO_2 absorption peaks and comparing the position to the reference calibrated positions, such that the wavenumber correction factor CF_v is given by:

(152) $$CF_v = \frac{v_{ref}}{v_{meas}} \quad \text{(Equation5)}$$

where v.sub.ref is the reference wavenumber and v.sub.meas is the measured drifted wavenumber. This can be based on the usual existence of CO_2 in the air with the amplified effect of the multi-pass gas cell.

(153) In another technique, a bandpass filter or a reference material can be inserted in the light path at a wavelength band away from the bands of interest. FIG. **38** is a diagram illustrating an example of a gas analyzer including a self-calibration component providing self-correction according to some aspects. The gas analyzer **3800** includes a gas cell **3802** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **3804** and **3806**, though other types of gas

cells may be used), optical coupling elements **3808** and **3810**, a light source **3812**, and a spectral sensor **3814** (e.g., spectrometer and associated detector). In a measurement mode of the gas analyzer **3800**, as shown in FIG. **38**, incident light **3816** produced by the light source **3812** may be coupled into the gas cell **3802** as input light via an input optical coupling element **3808** (e.g., an off-axis parabolic mirror). The input light **3816** may be reflected between the two reflectors **3804** and **3806** to cause light interaction with a sample (not shown) within the gas cell **3802**. Output light **3818** from the gas cell **3802** may be directed towards the spectral sensor **3814** via an output optical coupling element **3810** (e.g., an off-axis parabolic mirror) to obtain a sample spectrum of the sample.

(154) In the example shown in FIG. **38**, the self-calibration component includes bandpass filter **3820** (or reference material) configured to be inserted into a light path of the output light **3818**. For example, the bandpass filter **3820** may be coupled to a motor **3822** to insert the bandpass filter into the light path of the output light in a calibration mode (e.g., during self-correction) to produce corrected output light **3824**.

(155) FIG. **39** is a diagram illustrating another example of a gas analyzer including a self-calibration component providing self-correction according to some aspects. As in the example shown in FIG. **38**, the gas analyzer **3900** includes a gas cell **3902** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **3904** and **3906**, though other types of gas cells may be used), optical coupling elements **3908** and **3910**, a light source **3912**, and a spectral sensor **3914** (e.g., spectrometer and associated detector). In this example, the self-calibration component includes a bandpass filter or reference material **3916** that may be inserted into a reference path outside of the gas cell **3902**. For example, during calibration mode, the main optical coupling elements **3908** and **3910** may be coupled to an actuator **3918**. In this example, the actuator **3918** may be configured to move the main reflectors **3908** and **3910** away from the gas cell light path during calibration mode. In calibration mode, incident light **3920** produced by the light source **3912** may be directed through the filter/reference material **3916** to produce reference light **3922** coupled into the spectral sensor **3914**. Thus, in the example shown in FIG. **39**, self-correction can be integrated with a self-referencing architecture.

(156) FIG. **40** is a diagram illustrating an example of a gas analyzer including a self-calibration component providing self-referencing and self-correction according to some aspects. The gas analyzer **4000** includes a gas cell **4002** (e.g., a Herriot gas cell or modified/asymmetric Herriot gas cell including reflectors **4004** and **4006**, though other types of gas cells may be used), optical coupling elements **4008** and **4010**, a light source **4012**, and a spectral sensor **4014** (e.g., spectrometer and associated detector). Self-referencing may be provided by a self-calibration component that corresponds to redirecting optical elements (e.g., mirrors) **4016** and **4018** that may be inserted into a light path of the modified Herriot cell **4002** to produce a short optical path length. For example, the redirecting optical elements **4016** and **4018** may be inserted into the Herriot cell **4002** using a mechanical or electro-mechanical mechanism, similar to that described above in connection with FIGS. **20**A and **20**B. Thus, the redirecting optical elements **4016** and **4018** may be configured to operate in a calibration mode to receive incident light (input light) produced by the light source **4012** via an input optical coupling element **4008** and to redirect the input light through the Herriot gas cell **4002** without reflecting the light off either of the reflectors **4004** and **4006**. The resulting output light (e.g., reference light) **4022** may be directed towards the spectral sensor **4014** via an output optical coupling element **4010**, where a reference spectrum may be obtained.

(157) In the example shown in FIG. **40**, the reference measurement (reference spectrum) can be also used for self-correction measuring the reference bursts position. For example, the spectral sensor **4014** may include an interferometer **4024** that includes a beam splitter (BS) **4026**, flat mirror (M**1**) **4028** in one arm, and another mirror (M**2**) **4030** with two-levels, leading to two bursts at two reference positions that can be used for correction of the optical path difference axis of the sensor interferometer **4024** and consequently correcting the wavelength drifts.

(158) FIG. **41** is a diagram illustrating an example of spectra of volatile organic compounds. For example, VOCs spectra with 60 cm.sup.−1 resolution are shown in FIG. **41**. Multivariate analysis techniques can be used to detect and quantify the concentration of each VOC even if there is spectral overlap between them. A database associated with the AI engine (e.g., AI engine **312/412** shown in FIGS. **3** and **4**) can be a hybrid database built using both experimental and theoretical data. The theoretical data may be augmented by the synthesized spectral sensor characteristics. In some examples, partial least square (PLS) regression can be used as a linear model, while in other examples, a neural network can be used as a non-linear model.

(159) PLS is a multivariate analysis technique that can be used in FTIR spectroscopy to predict the concentrations of gases using their spectra. For example, the following procedure may be used: 1. VOCs spectra are simulated by different concentrations using the database of PNNL (these spectra are called the training set). 2. The simulated spectrum are fed to the PLS algorithm to generate a calibration model which can predict the concentrations from the spectra. 3. VOCs spectra are simulated again but with different concentrations that is in the range of the training set (these spectra are called the testing set). 4. Noise is then added to the testing set with the amplitude that guarantees the targeted signal-to-noise ratio (SNR) for the spectrometer. Other artifacts, such as baseline drifts, wavelength errors, and self-apodization can be added. 5. Concentrations of the testing set are then calculated using the PLS calibration model and then compared to the actual concentrations. 6. Different errors (RMS error, peak error, . . . etc.) can be calculated to evaluate the PLS calibration model.

(160) In an example, 35 gas spectra of VOCs were simulated (e.g., five simulations for every gas with different concentrations). No gas mixtures were required in preparing this calibration model. The simulation was made with signal-to-noise ratio (SNR) 20,000 and optical path length of 5 m and 15 m. Peak errors results from the PLS model are shown below in Table 1. The path length used (**L1**-**L2**) is 15 m and the SNR is 20000:1. A closer inspection of the values of the errors shows the following: 1) Formaldehyde error is the minimum because it has the strongest absorption among this group of VOCs, 2) The errors of aldehydes group is less than that of the BTEX group because the aldehydes have smaller overlapping compared to BTEX.

(161) TABLE-US-00001 TABLE 1 Gas Peak Error (µg/m.sup.3) Formaldehyde 5.3 Acetaldehyde 13.9 Toulene 79.5 Ethyl benzene 66.1 Styrene 60 Acrolein 35.2 Xylene 120.5

(162) Since some VOCs and gases in air are overlapped in the spectrum, in various aspects, a spectral resolution enhancement algorithm can be applied before the prediction occurs. This can be inside the AI engine or in a preceding block in the system. Examples of algorithms used include auto-regression, deep learning and neural network, compressive sensing FTIR, or any suitable super resolution algorithm.

(163) Within the present disclosure, the word "exemplary" is used to mean "serving as an example, instance, or illustration." Any implementation or aspect described herein as "exemplary" is not necessarily to be construed as preferred or advantageous over other aspects of the disclosure. Likewise, the term "aspects" does not require that all aspects of the disclosure include the discussed feature, advantage or mode of operation. The term "coupled" is used herein to refer to the direct or indirect coupling between two objects. For example, if object A physically touches object B, and object B touches object C, then objects A and C may still be considered coupled to one another— even if they do not directly physically touch each other. For instance, a first object may be coupled to a second object even though the first object is never directly physically in contact with the second object. The terms "circuit" and "circuitry" are used broadly, and intended to include both hardware implementations of electrical devices and conductors that, when connected and configured, enable the performance of the functions described in the present disclosure, without limitation as to the type of electronic circuits, as well as software implementations of information and instructions that, when executed by a processor, enable the performance of the functions described in the present disclosure.

(164) One or more of the components, steps, features and/or functions illustrated in FIGS. **1-41** may be rearranged and/or combined into a single component, step, feature or function or embodied in several components, steps, or functions. Additional elements, components, steps, and/or functions may also be added without departing from novel features disclosed herein. The apparatus, devices, and/or components illustrated in FIGS. **1-41** may be configured to perform one or more of the methods, features, or steps described herein. The novel algorithms described herein may also be efficiently implemented in software and/or embedded in hardware.

(165) It is to be understood that the specific order or hierarchy of steps in the methods disclosed is an illustration of exemplary processes. Based upon design preferences, it is understood that the specific order or hierarchy of steps in the methods may be rearranged. The accompanying method claims present elements of the various steps in a sample order, and are not meant to be limited to the specific order or hierarchy presented unless specifically recited therein.

(166) The previous description is provided to enable any person skilled in the art to practice the various aspects described herein. Various modifications to these aspects will be readily apparent to those skilled in the art, and the generic principles defined herein may be applied to other aspects. Thus, the claims are not intended to be limited to the aspects shown herein, but are to be accorded the full scope consistent with the language of the claims, wherein reference to an element in the singular is not intended to mean "one and only one" unless specifically so stated, but rather "one or more." Unless specifically stated otherwise, the term "some" refers to one or more. A phrase referring to "at least one of" a list of items refers to any combination of those items, including single members. As an example, "at least one of: a, b, or c" is intended to cover: a; b; c; a and b; a and c; b and c; and a, b and c. All structural and functional equivalents to the elements of the various aspects described throughout this disclosure that are known or later come to be known to those of ordinary skill in the art are expressly incorporated herein by reference and are intended to be encompassed by the claims. Moreover, nothing disclosed herein is intended to be dedicated to the public regardless of whether such disclosure is explicitly recited in the claims. No claim element is to be construed under the provisions of 35 U.S.C. § 112(f) unless the element is expressly recited using the phrase "means for" or, in the case of a method claim, the element is recited using the phrase "step for."

Claims

1. A gas analyzer, comprising: a light source configured to produce incident light; a gas cell configured to receive a sample, the gas cell further configured to receive input light corresponding to the incident light or an interference beam produced based on the incident light, the gas cell further configured to produce output light based on light interaction with the sample within the gas cell in a measurement mode; a spectral sensor comprising a spectrometer configured to receive the incident light from the light source or the output light from the gas cell and further configured to produce the interference beam, the interference beam corresponding to the input light or being produced based on the output light, the spectral sensor further comprising a detector configured to obtain a sample spectrum of the sample based on the interference beam; an artificial intelligence engine configured to receive the sample spectrum and to generate a result indicative of at least one parameter associated with the sample based on the sample spectrum; control circuitry configured to control the light source and the spectral sensor; and a self-calibration component configured to enable background reference calibration of the sample spectrum using a background spectrum to compensate for spectral drift of the gas analyzer in a spectral domain, wherein the self-calibration component is configured to obtain the background spectrum using the gas cell and without evacuating the sample from the gas cell.

2. The gas analyzer of claim 1, wherein the spectrometer comprises a micro-electro-mechanical systems (MEMS) interference device.

3. The gas analyzer of claim 1, wherein the gas cell comprises an asymmetric Herriot cell comprising a first reflector and a second reflector opposite the first reflector configured to produce multiple reflections of the input light therebetween, the first reflector and the second reflector comprising different radius of curvature.

4. The gas analyzer of claim 3, wherein the self-calibration component comprises redirecting optical elements inserted into a light path of the asymmetric Herriot gas cell and configured to operate in a calibration mode to receive the input light and to redirect the input light through the asymmetric Herriot gas cell without reflecting off the first reflector or the second reflector to obtain a reference spectrum.

5. The gas analyzer of claim 1, wherein the gas cell comprises a White gas cell comprising a plurality of reflectors and the self-calibration component comprises redirecting optical elements inserted into a light path of the White gas cell and configured to operate in a calibration mode to receive the input light and to redirect the input light through the gas cell without reflecting off any of the plurality of reflectors to obtain a reference spectrum.

6. The gas analyzer of claim 5, wherein the redirecting optical elements are mounted on a holder coupled to a stepper motor for insertion and removal of the redirecting optical elements into and out of the light path.

7. The gas analyzer of claim 5, wherein the redirecting optical elements are coupled to a hinge for insertion and removal of the redirecting optical element into and out of the light path.

8. The gas analyzer of claim 1, wherein the gas cell comprises a circular gas cell comprising a circular reflecting element and the self-calibration component comprises a flat mirror inserted into a light path within the circular gas cell and configured to operate in a calibration mode to receive the input light and to redirect the input light through the gas cell without reflecting off the circular reflecting element to obtain a reference spectrum.

9. The gas analyzer of claim 1, wherein the self-calibration component comprises a first external reflector and a second external reflector, each of the first external reflector and the second external reflector being outside of the gas cell and configured to operate in a calibration mode to receive the incident light and to produce reference light reflected towards the spectral sensor to obtain a reference spectrum without the sample.

10. The gas analyzer of claim 9, wherein the first external reflector and the second external reflector are movable mirrors coupled to an actuator configured to insert the moveable mirrors into a light path of the incident light to reflect the incident light to produce the reference light directed towards the spectral sensor in the calibration mode.

11. The gas analyzer of claim 9, further comprising: a reference cell configured to receive the incident light reflected from the first external reflector and to reflect the incident light towards the second external reflector to produce the reference light for reflection towards the spectral sensor.

12. The gas analyzer of claim 9, further comprising: a shutter configured to switch between the calibration mode and the measurement mode.

13. The gas analyzer of claim 12, further comprising: a beam combiner configured to combine the output light and the reference light for input to the spectral sensor to produce a combined spectrum in the calibration mode, the spectral sensor configured to extract the reference spectrum from the combined spectrum by subtracting the sample spectrum from the combined spectrum.

14. The gas analyzer of claim 9, further comprising: an electro-optic controlled element configured to switch between the calibration mode and the measurement mode.

15. The gas analyzer of claim 9, further comprising: an interferometer comprising an optical path difference between first and second light paths within the interferometer configured to switch between the calibration mode and the measurement mode.

16. The gas analyzer of claim 9, further comprising: a bandpass filter coupled between the first external reflector and the second external reflector configured to produce the reference light comprising reference bands for input to the spectral sensor; and a bandstop filter configured to

filter the reference bands from the input light for input to the gas cell.

17. The gas analyzer of claim 9, wherein the light source is a dual filament light source and the incident light comprises first input light directed to the gas cell and second input light directed to the first external reflector, the dual filament light source being further configured to switch between the first input light and the second input light.

18. The gas analyzer of claim 9, further comprising: an interferometer configured to receive the output light and the reference light and to produce a modulated light beam input to the spectral sensor, the interferometer comprising two arms and a two-level mirror in one of the two arms.

19. The gas analyzer of claim 1, wherein the self-calibration component comprises a moveable mirror within the gas cell configured to operate in the measurement mode at a first position of the moveable mirror and to operate in a calibration mode at a second position of the moveable mirror to receive the input light and to produce reference light reflected towards the spectral sensor to obtain a reference spectrum without the sample.

20. The gas analyzer of claim 1, wherein the gas cell comprises a toroidal gas cell comprising a single input/output and wherein the self-calibration component comprises: a solenoid attached to a reflective material and coupled to the single input/output, the solenoid configured to move the reflective material into a light path of the incident light in a calibration mode to couple the incident light to the spectral sensor without entering the toroidal gas cell to obtain a reference spectrum.

21. The gas analyzer of claim 1, wherein the self-calibration component is included within the AI engine.

22. The gas analyzer of claim 1, wherein the self-calibration component comprises a bandpass filter configured to be inserted into a light path of the output light.

23. The gas analyzer of claim 1, wherein the spectrometer comprises an interferometer comprising two arms and the self-calibration component comprises a two-level mirror in one of the two arms.

24. The gas analyzer of claim 1, further comprising: an atmospheric compensation unit configured to reduce an effect of the presence of one or more undesired substances in the gas cell.

25. The gas analyzer of claim 24, wherein the atmospheric compensation unit comprises one or more sensors configured to detect the one or more undesired substances and to produce sensor output fed into the AI engine, the AI engine configured to use the sensor output to produce the result.

26. The gas analyzer of claim 25, wherein the atmospheric compensation unit comprises an apodization function applied by the spectral sensor on an interferogram associated with the sample spectrum.

27. The gas analyzer **25**, wherein the atmospheric compensation unit comprises a database of absorption spectra of the one or more undesired substances, and the AI engine is configured to is configured to access the database to generate processed spectra based on the absorption spectra and to provide the processed spectra to the spectrometer, the spectrometer using the processed spectra to produce the sample spectrum.

28. The gas analyzer of claim 1, further comprising: a sample interface configured to input the sample into the gas cell.

29. The gas analyzer of claim 1, further comprising: at least one sensor configured to generate sensor data related to the sample and to provide the sensor data to the AI engine.

30. The gas analyzer of claim 1, wherein the AI engine comprises a cloud-based AI engine.

31. The gas analyzer of claim 1, wherein the spectral sensor comprises a thermal control unit configured to stabilize a temperature at the detector.