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Standard Practice for
Open-Path Fourier Transform Infrared (OP/FT-IR) Monitoring of Gases and Vapors in Air[1]

This standard is issued under the fixed designation E1982; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice covers procedures for using active open-path Fourier transform infrared (OP/FT-IR) monitors to measure the concentrations of gases and vapors in air. Procedures for choosing the instrumental parameters, initially operating the instrument, addressing logistical concerns, making ancillary measurements, selecting the monitoring path, acquiring data, analyzing the data, and performing quality control on the data are given. Because the logistics and data quality objectives of each OP/FT-IR monitoring program will be unique, standardized procedures for measuring the concentrations of specific gases are not explicitly set forth in this practice. Instead, general procedures that are applicable to all IR-active gases and vapors are described. These procedures can be used to develop standard operating procedures for specific OP/FT-IR monitoring applications.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 *This practice does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this practice to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.4 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]
E131 Terminology Relating to Molecular Spectroscopy
E168 Practices for General Techniques of Infrared Quantitative Analysis
E1421 Practice for Describing and Measuring Performance of Fourier Transform Mid-Infrared (FT-MIR) Spectrometers: Level Zero and Level One Tests
E1655 Practices for Infrared Multivariate Quantitative Analysis
E1685 Practice for Measuring the Change in Length of Bolts Using the Ultrasonic Pulse-Echo Technique

2.2 *Other Documents:*
FT-IR Open-Path Monitoring Guidance Document[3]
Compendium Method TO-16 Long-Path Open-Path Fourier Transform Infrared Monitoring of Atmospheric Gases[4]

3. Terminology

3.1 For definitions of terms used in this practice relating to general molecular spectroscopy, refer to Terminology E131.

3.2 For definitions of terms used in this practice relating to OP/FT-IR monitoring, refer to Practice E1685.

3.3 For definitions of general terms relating to optical remote sensing, refer to the FT-IR Open Path Monitoring Guidance Document.

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4. Significance and Use

4.1 An OP/FT-IR monitor can, in principle, measure the concentrations of all IR-active gases and vapors in the atmosphere. Detailed descriptions of OP/FT-IR systems and the fundamental aspects of their operation are given in Practice E1685 and the FT-IR Open-Path Monitoring Guidance Document. A method for processing OP/FT-IR data to obtain the concentrations of gases over a long, open path is given in Compendium Method TO-16. Applications of OP/FT-IR systems include monitoring for gases and vapors in ambient air, along the perimeter of an industrial facility, at hazardous waste sites and landfills, in response to accidental chemical spills or releases, and in workplace environments.

5. Instrumental Parameters

5.1 Several instrumental parameters must be chosen before data are collected with an OP/FT-IR system. These parameters include the measurement time, spectral resolution, apodization function, and zero filling factor. In some cases, the choice of these parameters might be limited by the parameters used to acquire and process the available reference spectra. Use the following procedures to select the instrumental parameters for each OP/FT-IR monitoring study.

5.2 *Measurement Time*—Determine the measurement time required to achieve the desired signal-to-noise ratio (S/N) at the selected resolution (see 5.3 and 6.7). Verify that this measurement time is appropriate for capturing the event being studied. If the measurement time is longer than the residence time of the plume in the path, the interferograms collected after the plume has exited the path will not contain spectral information from the target gas. Adding these signals in the interferogram domain to signals that contain information from the target gas will result in a dilution effect and can cause band distortions and nonlinearities. The variability in the water vapor concentration along the path can also limit the use of extensive signal averaging to improve the S/N. Measurement times from 1 min to 5 min are typical for ambient monitoring, whereas shorter measurement times may be required for plume modeling studies.

5.3 *Resolution*—The choice of what spectral resolution to use while collecting OP/FT-IR data depends on the spectral characteristics of the target gases, the measurement time required to observe the pollutant plume, the concentrations of the target gases, the presence of interfering species, the choice of analysis method, and the data quality objectives of the monitoring study. This choice might be limited by the capabilities of the specific OP/FT-IR monitor used to collect data. Most commercially available, portable OP⁄FT-IR monitors are capable of producing spectra at a maximum resolution of 0.5 cm^{-1} or 1 cm^{-1}, although instruments are available that will produce spectra at 0.125 cm^{-1} resolution. There is currently no consensus as to the optimum resolution to use while collecting field data. Most current practitioners use a resolution of either 0.5 cm^{-1} or 1.0 cm^{-1}, although recent advances in instrumentation and data analysis techniques provide for the potential of using much lower resolutions. The choice of resolution can also affect other decisions that the operator must make before collecting or analyzing the data. For example, the spectral resolution affects the type of background spectrum that can be used, the method for generating a water vapor reference spectrum, and the choice of analysis method. The following steps can be taken to choose the best resolution for a particular application.

5.3.1 Examine reference spectra of the target gases and potential interfering species. If possible, acquire or obtain reference spectra of these gases at various resolutions. Determine the lowest resolution that resolves the spectral features of interest. Use this resolution as a starting point for future measurements.

5.3.2 If the appropriate facilities are available, develop calibration curves of the target gases at different resolutions. If an inadequate resolution is used, the relationship between the peak absorbance and concentration will not be linear. This relationship is also affected by the apodization function (see 5.4). If the compound of interest does not respond linearly with respect to concentration, a correction curve must be applied to the data during quantitative analysis.

5.3.3 Determine the effect of resolution on the other procedures involved with generating OP/FT-IR data, such as the creation of a synthetic background spectrum (see 10.3) and a water vapor reference spectrum (see 10.6.1) from the field spectra. These procedures rely on a series of subjective judgements, which require a visual inspection of the field spectra. The use of a higher resolution generally facilitates the ability of the operator to visualize the pertinent features of the field spectra.

5.3.4 Assess the resolution requirements of the analysis method. If the comparison (see 10.8.1) or scaled subtraction (see 10.8.2) method is used, the resolution should be sufficient to separate the spectral features of the target gases from those of the interfering species. If classical least squares (CLS) is used (see 10.8.3), a resolution higher than 4 cm^{-1} is generally required [1].[5] If partial least squares (PLS) is used (see 10.8.3), a resolution as low as 16 cm^{-1} may be sufficient [2].

NOTE 1—Most volatile organic compounds of interest in OP/FT-IR monitoring applications have absorption envelopes with full widths at half heights (FWHHs) of approximately 20 cm^{-1}. This observation would indicate that low-resolution spectra would be adequate for OP/FT-IR measurements. However, each OP/FT-IR spectrum will also contain features due to ambient gases, such as water vapor, carbon dioxide, carbon monoxide, and methane, which have FWHHs on the order of 0.2 cm^{-1} at atmospheric pressure. If low resolution measurements are made, the analysis method must be able to handle the spectral overlap and nonlinearities caused by an inadequate resolution of these atmospheric gases.

5.4 *Apodization*—Use the same apodization function that was used to process the reference spectra. If a choice of apodization function can be made, the Norton-Beer-medium function typically yields the best representation of the true absorbance as compared to Happ-Genzel or triangular apodization.

5.5 *Zero Filling*—Assuming that the field spectra were acquired at the same resolution as the reference spectra, choose

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[5] The boldface numbers in parentheses refer to a list of references at the end of this standard.

zero-filling parameters that allow the data point density of the field spectra to match that of the reference spectra. In general, the original interferogram should be zero filled to the degree that the number of data points used in the Fourier transform is twice that in the original interferogram. No advantage is gained by zero filling by more than a factor of two for most applications.

6. Initial Instrument Operation

6.1 Several tests should be conducted before the OP/FT-IR monitor is deployed for a field study. These tests include measuring the electronic noise, the distance at which the detector saturates, the linearity of the system, the signal due to internal stray light or ambient radiation, the signal strength as a function of distance, and the random baseline noise. Use the instrumental parameters chosen in 5.2 through 5.5 for these tests.

6.2 *Measure the Electronic Noise*—Place a piece of opaque material in front of the detector element while the detector is operational, for example after the mercury-cadmium-telluride (MCT) detector has been cooled and has equilibrated. Record the signal either as the interferogram or as a single-beam spectrum with the detector blocked. This signal represents the electronic noise of the system. The magnitude of this signal should be less than 0.25 % of the signal without the detector blocked, remain relatively constant over time, and decrease with the square root of the measurement time. If this signal is uncharacteristically large, an electrical component is most likely producing spurious noise. When this is the case, service of the system is indicated.

6.3 *Measure the Distance to Detector Saturation*—The distance at which the detector becomes saturated determines the minimum pathlength over which quantitative data can be obtained without making changes to the instrument. Evidence of detector saturation indicates that the detector may not be responding linearly to changes in the incident light intensity.

6.3.1 Set up the OP/FT-IR system with the retroreflector (monostatic configuration) or external, active IR source (bistatic configuration) at some predetermined distance, for example, 25 m, from the receiving telescope.

6.3.2 Align the system to maximize the detector output, which can be measured either as the peak-to-peak voltage of the interferogram centerburst or the intensity of a specific wavenumber in the single-beam spectrum. If the intensity of the single-beam spectrum is used, choose a wavenumber region that does not contain any absorption bands due to the target gases or atmospheric gases, such as water vapor.

6.3.3 Obtain a single-beam spectrum.

6.3.4 Examine the single-beam spectrum in the wavenumber region below the detector cutoff frequency. The instrument response in this region should be flat and at the baseline. An elevated baseline in this wavenumber region is due to nonphysical energy and indicates that the detector is saturated. A test for determining the ratio of the nonphysical energy to the maximum energy in the single-beam spectrum is given in Practice E1421. An example of an OP/FT-IR spectrum that exhibits nonphysical energy is given in Practice E1685.

6.3.5 If nonphysical energy is observed in the single-beam spectrum obtained at the initial pathlength, increase the pathlength until the instrument response below the detector cutoff frequency is flat and at the baseline. This distance represents the minimum operating pathlength.

6.3.6 If the instrument response below the detector cutoff frequency is flat and at the baseline in the single-beam spectrum obtained at the initial pathlength, decrease the pathlength until nonphysical energy is observed in the single-beam spectrum. This distance represents the minimum operating pathlength.

6.3.7 If nonphysical energy is observed at the desired monitoring pathlength and the pathlength cannot be increased, attenuate the IR signal by placing a fine wire mesh screen in the modulated, collimated beam. Changing the gain of the detector preamplifier to lower the magnitude of the signal is not useful because the detector nonlinearity does not depend on gain.

NOTE 2—Determining the distance at which the detector becomes saturated is particularly important for MCT detectors. Detector saturation is not as severe a problem for thermal detectors, such as deuterated triglycine sulfate detectors.

6.4 *Linear Response*—There are two types of nonlinearity that can affect OP/FT-IR data: detector nonlinearity and nonlinearity in absorbance. Evidence of detector nonlinearity can be observed by conducting the tests described in 6.3, although the absence of nonphysical energy in the single-beam spectrum does not guarantee that the detector is operating linearly. Some MCT detectors exhibit nonlinear response even when there is no evidence of detector saturation. The OP/FT-IR system can also exhibit nonlinearity in the change in absorbance with respect to changes in concentration due to the convolution of the instrumental line shape function with the spectral data. The choice of apodization function affects the severity of this nonlinearity. If a multipoint calibration is used in the data analysis, this type of nonlinearity can be accounted for. However, many OP/FT-IR systems rely on a single-point calibration. When this type of calibration model is used, the absorbance of the reference spectra should match the absorbance of the field spectra as closely as possible. The linearity of the system can be checked by using one of the following methods: analyzing polymer films of different, known thicknesses; using a dual-chambered gas cell; or attenuating the beam with wire screens of different, known mesh sizes.

6.4.1 *Polymer Films*—Acquire spectra of polymer films of different thicknesses to test the linearity of the OP/FT-IR system.

6.4.1.1 Collect a single-beam spectrum over the monitoring path without the polymer film in the beam. Use this spectrum as the background spectrum.

6.4.1.2 Insert a polymer film of known thickness into the IR beam and obtain a single-beam spectrum. Create an absorption spectrum from this spectrum by using the background spectrum acquired in 6.4.1.1.

6.4.1.3 Replace the first polymer film with another film of a different, known thickness and obtain a single-beam spectrum. Create an absorption spectrum from this spectrum by using the background spectrum obtained in 6.4.1.1.

6.4.1.4 Measure the absorbance maxima of selected bands in the two absorption spectra acquired in 6.4.1.2 and 6.4.1.3. Choose absorption bands that are not saturated. Perform this test on several absorption bands in different regions of the spectrum.

6.4.1.5 Compare the absorbance value of the selected band in the spectrum of one polymer film to that measured in the other. The ratio of the absorbance values of the two different films should be equal to the ratio of the film thicknesses.

NOTE 3—If the thickness of the polymer film used to test the linearity of the system is not known it can be calculated by using Eq 1:

$$b = \frac{1}{2n} \frac{N}{(v_1 - v_2)} \qquad (1)$$

where:
b = thickness of the sample,
n = refractive index of the sample,
N = number of interference fringes in the spectral range from v_1 to v_2,
v_1 = first wavenumber in the spectral range over which the fringes are counted, and
v_2 = second wavenumber in the spectral range over which the fringes are counted.

6.4.2 *Dual-Chambered Gas Cell*—Use a dual-chambered gas cell containing a high concentration of the target gas to test the linearity of the system. This cell should be designed with two sample chambers that differ in length by a known amount and are coupled so that each chamber contains the same concentration of the target gas (3).

6.4.2.1 Fill the dual-chambered cell with dry nitrogen at atmospheric pressure and insert it into the IR beam.

6.4.2.2 Acquire a single-beam spectrum along the monitoring path. Use this spectrum as the background spectrum for the chamber that is in the IR beam.

6.4.2.3 Reposition the cell so that the other chamber is in the IR beam, and acquire a single-beam spectrum along the monitoring path. Use this spectrum as the background spectrum for that chamber.

6.4.2.4 Fill the cell with a high concentration of the target gas. The absolute concentration of the target gas does not need to be known with this method.

6.4.2.5 Acquire single-beam spectra alternatively with each chamber positioned in the IR beam. Create absorption spectra by using the appropriate background spectrum for each chamber.

6.4.2.6 Measure the absorbance maxima of selected bands in the two spectra created in 6.4.2.5. Choose absorption bands that are not saturated. Perform this test on several absorption bands in different regions of the spectrum.

6.4.2.7 Compare the absorbance value measured with one chamber to that measured with the other. The ratio of the absorbance values measured with the two separate chambers in the beam should be equal to the ratio of the lengths of the chambers.

6.4.3 *Wire Mesh Screens*—Insert a wire screen of a known mesh size in the IR beam and record the signal. Remove this wire screen, insert another screen of a different, known mesh size in the beam, and record the signal. The ratio of the signals obtained with the two different screens should be equal to the ratio of the mesh sizes of the screens.

NOTE 4—Linearization circuits are available to minimize the problem of detector nonlinearity. These linearization circuits may not perform adequately for all detectors.

6.5 *Measure the Signal Due to Internal Stray Light or Ambient Radiation*—Single-beam spectra recorded with an OP/FT-IR monitor can exhibit a non-zero response in wavenumber regions in which the atmosphere is totally opaque. If the detector has been determined to be responding linearly to changes in the incident light intensity, this non-zero response can be attributed to either internal stray light or ambient radiation. Internal stray light is most likely to be a problem in monostatic systems that use a single telescope to transmit and receive the IR beam. Ambient radiation mostly affects bistatic systems in which an unmodulated, active IR source is separated from the interferometer and detector. The presence of internal stray light or ambient radiation causes errors in the photometric accuracy and, ultimately, errors in the concentration measurements. The magnitude of the instrument response due to internal stray light or ambient radiation determines the minimum useful signal that can be measured with the OP/FT-IR system.

6.5.1 *Measure the Internal Stray Light*—In monostatic systems that use a single telescope to transmit and receive the IR beam, point the telescope away from the retroreflector or move the retroreflector out of the field of view of the telescope and collect a single-beam spectrum. This spectrum represents the internal stray light of the system and is independent of the pathlength. Record this spectrum at the beginning of each monitoring program or whenever optical components in the system are changed or realigned. An example of an internal stray light spectrum is given in Practice E1685.

NOTE 5—Internal stray light can also be caused by strong sources of IR radiation that are in the field of view of the instrument. For example, the sun may be in the instrument's field of view during sunrise or sunset and cause an unwanted signal from reflections inside the instrument.

6.5.2 *Measure the Ambient Radiation*—In bistatic systems, which use an unmodulated, active IR source that is separated from the interferometer and detector, block or turn off the source and collect a single-beam spectrum. This spectrum is a record of the IR radiation emitted by the objects in the field of view of the instrument. Because this spectrum depends on what objects are in the field of view, it also depends on the pathlength. Thus, the ambient radiation spectrum must be acquired each time the pathlength is changed or whenever different objects come into the field of view. A recommended schedule for recording the ambient radiation spectrum has not been determined for all situations. However, recording an ambient radiation spectrum once every half hour is typical for most applications. An example of an ambient radiation spectrum is given in Practice E1685.

NOTE 6—The ambient radiation spectrum recorded by an OP/FT-IR monitor is a composite of the various IR sources in the field of view of the instrument, such as gray body radiators, emission bands from molecules in the atmosphere, and the instrument itself. Because the ambient radiation spectrum is temperature dependent, its relative contribution to the total signal will vary. This variation will most likely be greater than any other source of instrumental noise. The ambient radiation spectrum will be different for each site and can also change with varying meteorological conditions throughout the day. For example, cloud cover can attenuate the

atmospheric emission bands.

6.6 *Measure the Signal Strength as a Function of Pathlength*—In OP/FT-IR systems, the IR beam is collimated before it is transmitted along the path, but diverges as it traverses the path. Once the diameter of the beam is larger than the retroreflector (monostatic system) or the receiving telescope (bistatic system), the signal strength will diminish as the square of the pathlength.

6.6.1 Start with the retroreflector or the external IR source at the minimum pathlength as determined in 6.3. Record the magnitude of the signal either as the peak-to-peak voltage of the interferogram centerburst or as the intensity of the single-beam spectrum at a specific wavenumber. Once the initial measurement has been recorded, move the retroreflector or IR source some distance away from the receiving telescope, for example, 25 m, and record the magnitude of the signal. Continue this procedure until the signal decreases as the square of the monitoring pathlength. Extrapolate the data to determine the distance at which the magnitude of the signal will reach that of the random noise (see 6.7), internal stray light, or ambient radiation. This distance represents the maximum pathlength for that particular OP/FT-IR monitor.

Note 7—In bistatic systems, the relative contribution of the ambient radiation to the total signal increases as the signal from the active IR source decreases. As the signal from the active IR source approaches zero, there may be apparent shifts in the peak intensity of the single-beam spectrum.

6.7 *Determine the Random Baseline Noise of the System*—Set up the instrument at a pathlength that is representative of that to be used during the field study. Collect two single-beam spectra sequentially. Do not allow any time to elapse between the acquisition of these two spectra. Create an absorption spectrum from these two spectra by using one spectrum as a background spectrum. Which spectrum is used for the background is not important. Measure the random noise as the root-mean-square (RMS) noise (4). The actual wavenumber range over which the noise should be calculated will vary with the number of data points per wavenumber in the spectrum. A range of 98 data points is optimum for the RMS noise calculation. The RMS noise should be determined in wavenumber regions that are not significantly impacted by water vapor, for example, 958 cm^{-1} to 1008 cm^{-1}, 2480 cm^{-1} to 2530 cm^{-1}, and 4375 cm^{-1} to 4425 cm^{-1}. Record the value of the RMS noise for future reference.

7. Logistical Concerns and Ancillary Measurements at the Monitoring Sites

7.1 *Logistical Concerns*—Several logistical concerns must be addressed at each monitoring site before the OP/FT-IR monitor is deployed in the field. Consideration must be given to power requirements, mounting and support requirements, and climate control. Some ancillary measurements should also be made.

7.1.1 *Power*—Supply the required electrical power to the spectrometer. In bistatic systems with a remote IR source, an additional source of power must be provided if an electrical outlet is not available. Some IR sources can operate off a portable 12 V power supply, such as a car or marine battery. The output of the battery must be stabilized for quantitative measurements.

7.1.2 *Mounting and Support*—For short-term field studies, the spectrometer, the retroreflector, or the remote IR source are typically mounted on transportable tripods with swivel heads that allow for vertical and horizontal adjustments. For permanent installations, a more rigid mounting system can be used. In either case, the OP/FT-IR monitor should be isolated from vibrations.

7.1.3 *Climate Control*—Although some OP/FT-IR systems might be designed to withstand the elements, some effort should be made to protect the optical and electrical components of the system from rain and other forms of moisture, corrosive gases, and extreme cold or heat.

7.1.3.1 Spectrometers with hygroscopic internal optics, such as KBr beamsplitter, must be purged with a dry, inert gas or hermetically sealed to prevent moisture from damaging the optics. As an alternative, ZnSe optical components can be used.

7.1.3.2 Water vapor can condense on optical components, such as the retroreflector, that are exposed to the atmosphere. Some method to prevent this condensation, such as heating the component slightly above the dew point, must be implemented.

7.1.3.3 If exposure of the optical components to a corrosive environment cannot be avoided, devise some type of system to purge the surface of the optical components to minimize this exposure.

7.1.3.4 The spectral response of the spectrometer can be sensitive to changes in ambient temperature. In some instruments, the interferometer will not scan at ambient temperatures below 5 °C. In permanent installations, the temperature inside the shelter that houses the spectrometer should be controlled and monitored. For short-term field studies conducted in cold-weather climates, the spectrometer should be covered with some type of heated, insulating material.

7.2 *Ancillary Measurements*—Make continuous, real-time measurements of the following parameters: temperature, relative humidity, barometric pressure, and wind velocity. These measurements should be recorded and archived with some type of automated data logger. Guidance for selecting and setting up the instruments for making meteorological measurements is given in a United States Environmental Protection Agency (USEPA) handbook (5). Although this handbook does not directly address open-path measurements, it provides useful information about meteorological instrumentation and measurements.

Note 8—A measurement of relative humidity is not satisfactory for use in OP/FT-IR monitoring. The actual partial pressure of water vapor must be determined. If relative humidity is measured, then the temperature must also be recorded so that the partial pressure of water can be calculated by consulting the Smithsonian psychrometric tables. These tables can be found in the *Handbook of Chemistry and Physics* (6).

8. Selecting the Monitoring Path

8.1 The monitoring path can be selected once the location of the pollutant source is known, pertinent meteorological data are available, and specific target gases have been chosen for the monitoring program.

8.2 *Orient the Path*—Determine the direction of the prevailing winds. Set up the monitoring path downward of the pollutant source and perpendicular to the wind field. Unless there is a specific need to do otherwise, the path should be horizontal to the ground because the concentration contours of the target gases can vary with altitude. An example of a possible orientation of the monitoring path relative to the pollutant source area is given in Fig. 1.

NOTE 9—The USEPA has amended Part 58 of Chapter 1 of Title 40 of the Code of Federal Regulations (40 CFR58) that define ambient air monitoring criteria for open-path monitors (7). These amendments describe how the path is to be chosen with respect to obstructions and height above the ground. They also describe the appropriate positioning of the path in relation to buildings, stacks, and roadways.

8.3 *Select the Pathlength*—Choose the pathlength to maximize the percentage of the plume from the pollutant source that is interrogated by the IR beam. The pathlength should be nominally longer than the width of the plume to account for variations in the plume over time. For homogeneously distributed gases, the path can be made longer, if needed, to increase the measured absorbance. For plumes of finite extent, making the path longer than the width of the plume is detrimental because the OP/FT-IR monitor measures the path-averaged concentration. If part of the path has zero concentration, then there is a dilution effect. In some applications, the pathlength might be determined by logistical concerns, such as the availability of electrical power and suitable sites to accommodate the instrument and peripherals.

NOTE 10—The actual dimensions of the plume are difficult to define. Some models assume that the concentration profile of the plume can be described by a Gaussian function. The boundaries of the plume, however, may not be known prior to selecting the monitoring path.
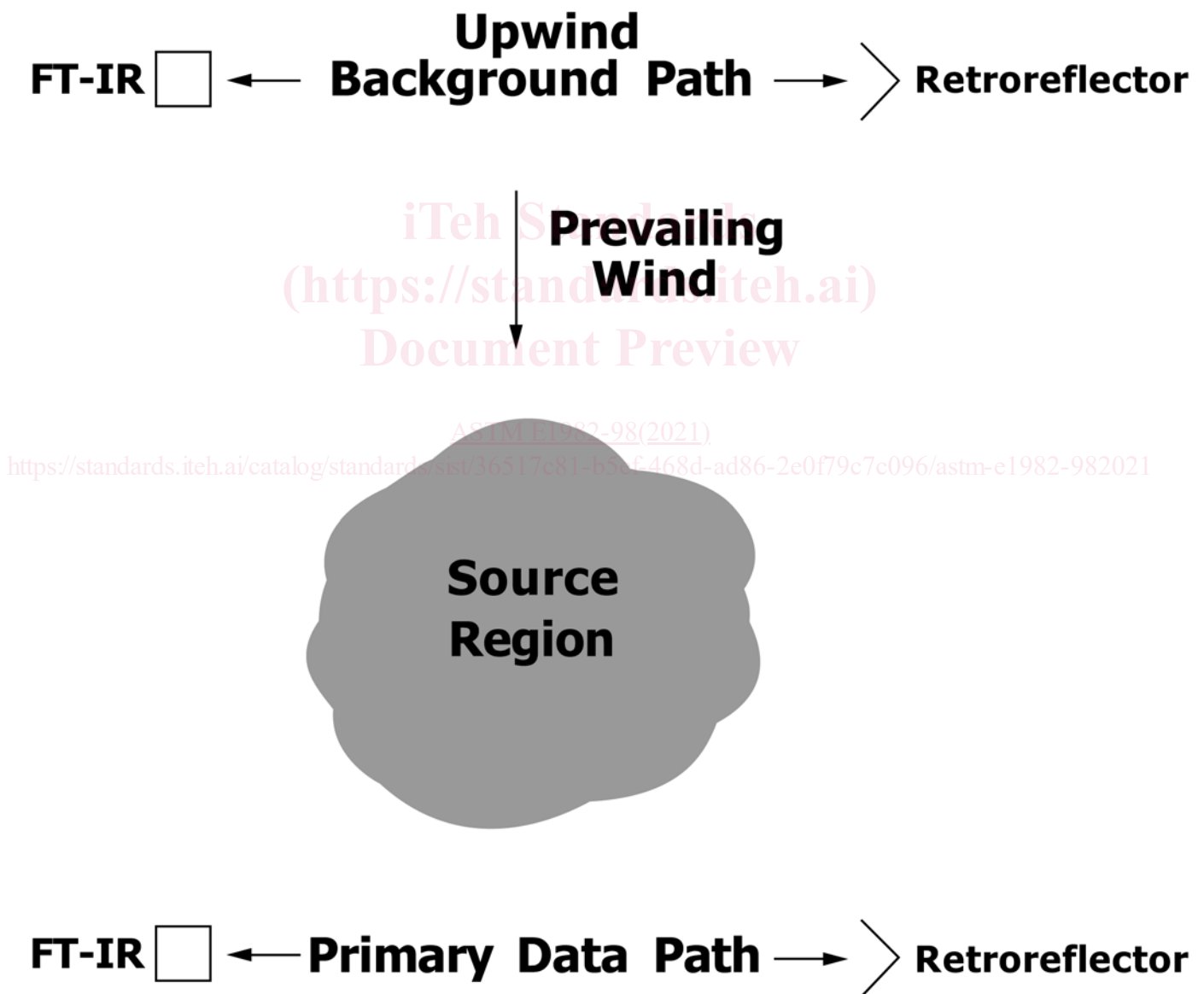

FIG. 1 Possible Orientations of the Monitoring Paths Relative to the Direction of the Prevailing Wind and the Pollutant Source for Primary Data Collection and for an Upwind Background Spectrum

8.3.1 *The Longest Pathlength*—The longest pathlength for a particular OP/FT-IR system was determined in 6.6.1 as the distance at which the total signal approaches the signal due to the system noise, internal stray light, or ambient radiation. For target gases and interfering species that are distributed homogeneously along the path, the atmosphere is optically dense at some pathlength. This distance represents the maximum pathlength for that gas and can be determined as follows.

8.3.1.1 Measure the absorbance of the analytical band of the target gas or interfering species from a reference spectrum. See 10.2 for procedures for choosing an analytical band. Record the concentration—pathlength product at which the reference spectrum was taken.

8.3.1.2 Calculate the absorptivity, *a*, for this gas by using Eq 2.

$$a = A_{ref}/b_{ref}C_{ref} \tag{2}$$

where:

A_{ref} = absorbance of the reference spectrum at a specified wavenumber,

b_{ref} = pathlength at which the reference spectrum was measured, and

c_{ref} = concentration of the reference standard.

8.3.1.3 Estimate the concentration of the target gas or interfering species from preexisting monitoring data or from ancillary measurements.

8.3.1.4 Select a maximum allowable absorbance value, based on the requirements of the analysis method.

8.3.1.5 Use Eq 3 to estimate the pathlength that would yield the maximum allowable absorbance value at the estimated concentration.

$$b_{max} = A_{max}/ac_{est} \tag{3}$$

where:

A_{max} = the maximum allowable absorbance selected in 8.3.1.4,

c_{est} = the concentration estimated in 8.3.1.3, and

a = the absorptivity calculated in 8.3.1.2.

The value of b_{max} calculated in Eq 3 is the longest allowable pathlength for measuring that particular target gas or interfering species.

8.3.2 *The Shortest Pathlength*—The shortest pathlength may be dictated by the distance at which the detector becomes saturated as determined in 6.3. If the instrument is operating linearly at any potential pathlength, the shortest pathlength for the target gas can be calculated as follows.

8.3.2.1 Measure the absorbance of the analytical band of the target gas from a reference spectrum. Record the concentration—pathlength product at which this spectrum was taken.

8.3.2.2 Calculate the absorptivity, a, for this gas by using Eq 2.

8.3.2.3 Estimate a minimum concentration that will be measured.

8.3.2.4 Set the minimum detectable absorbance at three times the RMS baseline noise as measured under normal operating conditions (see 6.7).

8.3.2.5 Calculate the minimum pathlength by using Eq 3, and the values of the absorptivity, minimum concentration, and minimum detectable absorbance found in 8.3.2.2 through 8.3.2.4, respectively.

8.4 *Estimate Detection Limits*—The method detection limit (MDL) in units of the concentration—pathlength product, for example ppm-m, can be estimated by using Eq 4.

$$(bc)_{min} = A_{min}/a \tag{4}$$

where:

A_{min} = minimum detectable absorbance, for example, three times the RMS baseline noise, and

a = the absorptivity, as calculated in 8.3.1.2.

To obtain the MDL of homogeneously distributed gases in units of concentration, for example ppb, divide the value of $(bc)_{min}$ by the pathlength. Examples of estimated detection limits for several hazardous air pollutants and common atmospheric gases are given in Annex A1 (see Table A1.1). This table can be used during the planning phase of a field study to determine if measurements of selected target gases are feasible at a particular monitoring site for a given monitoring pathlength. This procedure is also applicable to estimating the MDL for the comparison (see 10.8.1) or the scaled subtraction (see 10.8.2) analysis methods. Lower estimates of the MDL may be obtained when mulivariate analysis methods (see 10.8.3) are used by calculating the standard error of measurement for the target gas in a spectrum in which the target gas is not present.

9. Data Acquisition

9.1 Perform the following steps to acquire the OP/FT-IR spectral data once the instrumental parameters have been chosen (see Section 5), initial performance tests have been completed (see Section 6), logistical concerns have been addressed (see Section 7), and the monitoring path has been selected (see Section 8).

9.2 *Align the Instrument*—Allow the system to equilibrate. Adjust the vertical and horizontal position of the receiving telescope, the retroreflector, or the external IR source to maximize the peak-to-peak voltage of the interferogram centerburst or the intensity of the single-beam spectrum at a specific wavenumber. Record the value of the maximum signal.

9.3 *Determine the Random Baseline Noise of the System*—Record the magnitude of the RMS noise as described in 6.7. Compare this value with historical data to determine that the instrument is performing within the data quality objectives of the study.

9.4 *Choose the Type of Data File*—Select the type of data file that is to be collected, for example, either a single-beam spectrum or an interferogram.

NOTE 11—The interferogram should be the type of raw data that is collected to allow for more choices in post-data acquisition processing.

9.5 *Acquire the Spectral Data*—Choose the number of data files to be collected and the intervals at which they are to be acquired, then start acquiring the data.