

# Sizing Chemical Flow Rates for Infrared Imaging Spectrometers

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## Abstract

For many years now, the Imaging Spectroscopy Department at The Aerospace Corporation has been releasing chemicals into the atmosphere at accurately measured rates, producing chemical plumes for infrared hyperspectral imaging spectrometers. The purpose is often to determine how well such a spectrometer and its software can identify the chemicals in the plume and determine the rate at which each chemical is being released. We are often asked to release a chemical at a rate that is barely detectable or at some multiple of that rate. The minimum detectable release rate does not have a fixed value; rather it varies with background temperature, wind speed, and air temperature, all of which we measure before every release. For an infrared imaging spectrometer viewing a plume from the ground against the sky, the background temperature is the sky radiometric temperature; when airborne and viewing ground, the background temperature is the ground radiometric temperature. In this report, a simple, approximate, but acceptably accurate equation is derived that shows how the expected minimum detectable release rate (or some multiple of it) varies with background radiometric temperature, wind speed, air temperature, and sampling distance (which depends on the field of view of the spectrometer and its distance from the plume). This approximate equation is derived for a downward-looking airborne imaging spectrometer but can be adapted to situations in which the imaging spectrometer is ground-based and the background is sky, trees, or any other object.

The derivation of this equation, which is used exclusively for sizing (that is, setting) chemical flow rates, includes a description of how a hyperspectral infrared imaging spectrometer detects a chemical plume, during the day or night, using only the natural infrared radiation present in the scene. There is no discussion, however, of the mathematical methods used to extract chemical release rates from an infrared imaging spectrometer's quantitative measurements.

## **Acknowledgement**

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# 1. Overview and Concepts

## 1.1 Introduction

For more than a decade, The Aerospace Corporation’s Imaging Spectroscopy Department has been discharging chemicals into the atmosphere at precisely measured rates into the field of view of a variety of hyperspectral imaging spectrometers. Usually, the discharge lasts at least a minute or two, producing a chemical plume, that is detected by the imaging spectrometer. Plume detection is termed “passive” because detection is made using only the natural radiation present; there are no active sources of radiation, such as a laser. Gases are typically released at a height between 25 and 50 ft through a tube whose diameter is 1 inch or less. Liquids are released through an atomizer as a fine mist. For a fairly volatile chemical, the mist will completely vaporize within a few meters downwind from the release point. Our releases, both liquid and gas, can be considered as point-source releases. Imaging spectrometers are used not only to detect the chemical plume and identify the chemicals in it, but also to make quantitative estimates of chemical flow rates, which can be compared to the measured rates.

## 1.2 Equation for Sizing Chemical Flow Rates

Aerospace is often asked to release a gas at a rate that is barely detectable (termed the minimum detectable quantity, or MDQ). At other times, we are asked to release at a rate  $S$  times MDQ, where  $S$  might range from 0.5 to 10. The minimum detectable quantity is not a fixed number, but rather depends on (1)  $u$ , the wind speed, (2)  $\Delta T$ , the magnitude of the difference between the air temperature and the background radiometric temperature, and (3)  $L$ , the sampling distance. The formula that we use to size the MDQ chemical release rate,  $q$ , is

$$q = Sq_0(u/u_0)(\Delta T_0/\Delta T)(L/L_0) \tag{1}$$

where  $q_0$  is the minimum detectable quantity when the wind speed =  $u_0$ ,  $\Delta T = \Delta T_0$ , and the sampling distance =  $L_0$ . Equation 1 is valid when the chemical plume underfills the pixel.

## 1.3 Meaning of Underfilled Pixel

Figure 1 illustrates what is meant by the plume underfilling the pixel. [The term “pixel” should refer to an element in an image (in this case, the image produced by an infrared imaging spectrometer); however, sometimes the area on the ground that is imaged onto a single pixel is also referred to as a “pixel” for lack of a better word.]

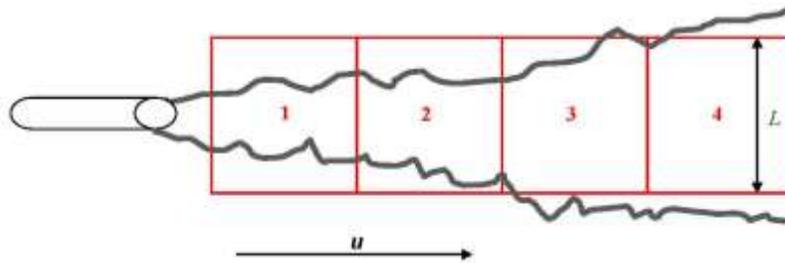


Figure 1. This diagram illustrates what is meant by a plume underfilling and overfilling a pixel. The double arrow labeled  $L$  is the ground sampling distance; the arrow labeled  $u$  points in the direction of the wind.

In Figure 1, a gas containing one or more chemicals that absorb and emit infrared radiation is being discharged into the atmosphere through a tube (or an exhaust stack, or a tailpipe) at a steady rate. For ease of discussion, let us consider the case where the plume is being observed by a downward-looking,

airborne, imaging spectrometer, viewing a flat, horizontal surface (e.g., ground) at an angle that is perpendicular to the surface. The area between the black lines in Fig. 1 would then represent the exhaust plume as viewed from above. The plume increases in size downwind as it turbulently entrains ambient air. Each of the numbered red squares represents the area on the ground imaged as a single pixel. The plume underfills pixels 1 and 2, and it overfills pixel 4. Pixel 3 is an intermediate case. The area imaged into a single pixel could, of course, be much larger relative to the exhaust tube than is shown here. Or if the area imaged in each pixel should be unusually small, the numbered red squares could represent, say, four adjacent pixels.

Suppose, for sake of discussion, that the surface over which the plume is passing is uniform in temperature and composition, so that the infrared spectrum of each of the four pixels shown in Figure 1 would be essentially identical if a plume were not present. Moreover, if at any instant, the plume temperature and the wind speed are the same in each pixel, then, ignoring turbulent fluctuations, the infrared signature of the chemicals in the plume would be identical for pixels 1 and 2, provided the plume is everywhere optically thin, which in most scenarios would be almost certainly the case, except perhaps right at the end of the exhaust tube, before the plume has entrained hardly any ambient air and grown in size. The infrared signature of the plume would be weaker in pixel 3 than in pixels 1 and 2, and still weaker in pixel 4, because there are fewer infrared-absorbing molecules in these pixels. As the distance from the aircraft to the plume is much greater than the distance from the plume to the ground, the ground and the plume can be considered to be in the same image plane, and the sampling distance  $L$  shown in Fig. 1 can accurately be termed the “ground sampling distance.”

In Eq. 1,  $q_0$  is set equal to the chemical’s minimum detectable quantity or MDQ. A chemical’s MDQ is, of course, different for different imaging spectrometers. A chemical’s MDQ also depends on the background scene against which its plume is observed; for example, the MDQ of a chemical plume against the sky is different from the MDQ of the same chemical’s plume viewed against the ground. Furthermore, a chemical’s MDQ varies with the nature of the ground, in particular, whether the ground is grassland, forest, desert, urban, light industrial, or heavy industrial. Kerry Buckland and others at The Aerospace Corporation have developed an algorithm for calculating a chemical’s MDQ using, among other things, that chemical’s quantitative laboratory infrared spectrum. Those calculated MDQs compare favorably (within experimental uncertainties) to MDQs determined from spectra taken by airborne infrared imaging spectrometers of chemical plumes of known flow rates. Measurements made by imaging spectrometers also show that Equation 1, when used to size the chemical flow rates, is acceptably accurate, and there is no obvious reason why Equation 1 needs to be modified. The aim of this report is to derive Equation 1 and explain why it is accurate enough for its purpose of sizing chemical flow rates.

Equation 1 will be derived by examining how the detectability of the plume in a single underfilled pixel, such as pixel 1 in Figure 1, changes with wind speed  $u$ , air temperature  $T_{\text{air}}$ , ground radiometric temperature  $T_{\text{grnd}}$ , and ground sampling distance  $L$ . The detectability of the plume in pixel 2 will obviously change in the same way. In general, the greater the number of pixels a barely detectable plume can be detected in, the more accurate the determination of its flow rate. Equation 1 gives no information about the accuracy of  $q_0$ ; it only predicts how the minimum detectable flow rate  $q$  changes with  $u$ ,  $\Delta T$ , and  $L$  for underfilled pixels.

#### 1.4 Qualitative Discussion of Plume Detection

When light enters an imaging spectrometer, it is dispersed by a prism or grating onto a detector array. In a hyperspectral imaging spectrometer, the photons that strike any detector element in the array are of nearly the same wavelength.

Consider a single detector element that receives infrared radiation of wavelength  $\lambda$ , where  $\lambda$  is in either the mid-wave or long-wave atmospheric window. Suppose that this detector element is viewing one of the pixels in Figure 1. If the plume shown in this figure were absent, this detector would receive infrared radiation only from the ground. Contributions from infrared active molecules always present in the atmosphere, such as carbon dioxide and water, are ignored in this discussion, inasmuch as  $\lambda$  is in an atmospheric window where these contributions can be small and are moreover accounted for in the determination of  $q_0$ . When the plume passes over the area imaged by the detector element that receives radiation of wavelength  $\lambda$ , the radiant flux from that area can change, either increasing or decreasing, if molecules in the plume absorb and emit infrared radiation at wavelength  $\lambda$ . If the ground radiometric temperature is higher than the temperature of the air in the plume, absorption will dominate over emission and the radiant flux on the detector will decrease from the value it would have had if the plume had not been present. Conversely, if the ground radiometric temperature is lower than the plume temperature, emission will dominate over absorption, and the radiant flux on the detector will increase.

## 1.5 Radiometric Temperature

Equation 1 requires a knowledge of  $\Delta T$ , which for an airborne imaging spectrometer is the magnitude of the difference between the plume temperature  $T_{\text{plume}}$  and the ground radiometric temperature  $T_{\text{grnd}}$ . In most cases, the plume temperature equals the surrounding air temperature  $T_{\text{air}}$ ; so, in terms of the measured temperatures,

$$\Delta T = |T_{\text{air}} - T_{\text{grnd}}| \quad (2)$$

The radiometric temperature is the temperature displayed by a radiometer when the emissivity of the object under view is set to 1.000. A radiometer measures the radiant flux over some range of wavelengths and from this measurement computes the temperature a blackbody would have to have to produce the measured radiant flux. The radiant flux from the object consists of its own thermal radiation and reflected radiation from its surroundings, which would include reflected radiation from the sky and from nearby buildings and trees. The radiometric temperature is also termed the “brightness temperature.” (Radiance was once termed “brightness.”) However, the use of the term brightness temperature can be ambiguous as sometimes (in Wikipedia, for example) it is defined as the temperature measured or calculated under conditions where reflected radiation is unimportant or is subtracted out.

We have radiometers that measure temperature over the following wavelength ranges: 3.4–4.2  $\mu\text{m}$ , 4.6–5.0  $\mu\text{m}$ , 8.05–12.7  $\mu\text{m}$ , 9.6–11.5  $\mu\text{m}$ , and 8.0–14  $\mu\text{m}$ . Although it is likely that the ground’s emissivity and reflectivity would vary over each of these wavelength bands, the measured average  $T_{\text{grnd}}$  is used for all wavelengths within the band.

For a more complete description of the radiometers that we use in our chemical releases and a description of the other equipment and procedures used, see Westberg and Matic 2016 [1].

## 1.6 Radiant Flux on a Detector Element

In this section, a formula is presented for the radiant flux  $\Phi_{\lambda,b}$  onto a detector element when there is no plume present. [The SI unit for radiant flux is watts.] A subscript  $\lambda$  is appended to the symbol  $\Phi_{\lambda,b}$  to indicate that this radiant flux can be different at different wavelengths; the subscript b stands for “background” since  $\Phi_{\lambda,b}$  can be considered the background flux. A formula is then given for the radiant flux  $\Phi_{\lambda,op}$  on a detector element from a plume that overfills the pixel and completely absorbs all the radiation at wavelength  $\lambda$  from the ground. The subscript op here stands for opaque plume. This section

ends with a discussion on how  $\Phi_{\lambda,op}$  and  $\Phi_{\lambda,b}$  are related to  $\Delta\Phi_{\lambda}$  where  $\Delta\Phi_{\lambda}$  is the change in the radiant flux on a detector element produced by a plume that is not necessarily opaque.

If the plume is absent, or is so dilute that it is well below the detection limit at wavelength  $\lambda$ , the radiant flux  $\Phi_{\lambda,b}$  on a single detector element would be proportional to the spectral radiance from the area on the ground that is in the detector element's field of view

$$\Phi_{\lambda,b} = aB_{\lambda}(T_{\text{grnd}}) \quad (3)$$

where  $a$  is the proportionality constant, which depends only on the properties of the spectrometer, not on the sources of radiation outside the spectrometer. In a simplified model for the spectrometer's responsivity,  $a$  might be proportional to the product of  $\Delta\lambda$ , the wavelength range of the radiation that falls on the detector element, and the fraction of the radiation that enters the spectrometer that is transmitted to the detector element.  $B_{\lambda}(T_{\text{grnd}})$  is the blackbody spectral radiance at radiometric temperature  $T_{\text{grnd}}$  and wavelength  $\lambda$ .

If the plume overfills the pixel and is opaque at wavelength  $\lambda$ , then the detector element will not receive any radiation at wavelength  $\lambda$  from the ground; all the radiation at this wavelength will be from the plume. The radiant flux  $\Phi_{\lambda,op}$  from an opaque plume is

$$\Phi_{\lambda,op} = aB_{\lambda}(T_{\text{air}}) \quad (4)$$

Equation 4 correctly implies that the air temperature within a plume can be determined by measuring the spectral radiance of an opaque plume, provided the constant  $a$  has been independently determined. A chemical plume is detected by the change it produces in the radiant flux. The maximum change possible is the absolute value of  $[\Phi_{\lambda,op} - \Phi_{\lambda,b}]$ , which is the change produced when the plume overfills the pixel and is opaque. A plume that is not opaque will produce some fraction  $f_{\lambda}$  of the maximum possible change

$$\Delta\Phi_{\lambda} = f_{\lambda} [\Phi_{\lambda,op} - \Phi_{\lambda,b}] = f_{\lambda} a [B_{\lambda}(T_{\text{air}}) - B_{\lambda}(T_{\text{grnd}})], \text{ where } 0 \leq f_{\lambda} \leq 1 \quad (5)$$

Equation 5 clearly implies that when  $T_{\text{air}} = T_{\text{grnd}}$ , the chemical plume will produce no change in the radiant flux on the detector element. Furthermore, because  $B_{\lambda}(T)$  is a monotonically increasing function of temperature, Eq. 5 also implies that when  $T_{\text{grnd}} > T_{\text{air}}$ , the plume will absorb more radiation than it will emit, leading to a reduction in the amount of radiant flux on the detector. Inversely, if the temperature of the air is greater than the ground radiometric temperature, emission will dominate over absorption, and the plume will produce an increase in the radiant flux on the detector.

## 2. A Simple Equation for Sizing Chemical Flows

### 2.1 Derivation

To derive Equation 1, the equation used to size (that is, set) the chemical flow rate, we need to make the following approximation, which is accurate for small values of  $\Delta T$

$$\left| B_{\lambda}(T_{\text{air}}) - B_{\lambda}(T_{\text{grnd}}) \right| = \frac{\partial B_{\lambda}}{\partial T} \left| (T_{\text{air}} - T_{\text{grnd}}) \right| = \frac{\partial B_{\lambda}}{\partial T} \Delta T \quad (6)$$

Also, to derive Equation 1,  $f_{\lambda}$  needs to be expressed in terms of mass flow rate  $q$ . The change in radiant flux  $\Delta\Phi_{\lambda}$  on a detector element due to an infrared absorbing plume can be expressed in words as

$$\Delta\Phi_{\lambda} = \begin{array}{l} \text{the change in radiant flux due to emission from the plume } plus \\ \text{the change in radiant flux from the ground due to absorption by the plume.} \end{array}$$

For an optically thin plume, Kirchhoff's law of thermal radiation and Beer's law of absorption give

$$\begin{array}{l} \text{change in radiant flux due to emission from the plume} = a\kappa_{\lambda}\bar{c}lB_{\lambda}(T_{\text{air}}) \\ \text{change in radiant flux from the ground due to absorption by the plume} = -a\kappa_{\lambda}\bar{c}lB_{\lambda}(T_{\text{grnd}}) \end{array}$$

where  $a$  is the proportionality constant defined and used in Eqs. 3 and 4,  $\kappa_{\lambda}$  is the molar absorption coefficient (base  $e$ ) of the chemical of interest, and  $\bar{c}l$  is the column abundance of this chemical in the plume and in the field of view of detector. Consequently,

$$\Delta\Phi_{\lambda} = a\kappa_{\lambda}\bar{c}l \left[ B_{\lambda}(T_{\text{air}}) - B_{\lambda}(T_{\text{grnd}}) \right] \quad (\text{optically thin plume})$$

Comparing the above equation to Equation 5 gives an expression for  $f_{\lambda}$

$$f_{\lambda} = \kappa_{\lambda}\bar{c}l \quad (\text{optically thin plume}) \quad (7)$$

Equation 7 is valid for any wavelength  $\lambda$  absorbed by the molecules in the plume, that is, any wavelength for which  $\kappa_{\lambda}$  is not zero.

The SI unit for the molar absorption coefficient  $\kappa_{\lambda}$  is  $\text{m}^2/\text{mol}$ . Physicists often use the unit  $\text{m}^2/\text{molecule}$  for  $\kappa_{\lambda}$  and give it the symbol  $\sigma$  and call it the absorption cross-section. The SI unit for column abundance  $\bar{c}l$  is  $\text{mol}/\text{m}^2$ . Often, column densities are used instead of column abundances. The usual unit for column density is  $\text{mg}/\text{m}^2$ .

There is no commonly used symbol for column abundance. The column abundance of a chemical is the average concentration  $\bar{c}$  of the chemical in a column (or prism) of constant cross-sectional area times the length  $l$  of the column. In the laboratory, the column is often a tube, and the chemical concentration is uniform within that tube; consequently, the column abundance would be written as  $cl$ . In a plume, there are, of course, no tubes. The column of interest in a plume must include all molecules of interest that at any moment are in the field of view of a detector on board an aircraft and exclude all molecules outside its field of view. Such a column would be a pyramid whose apex is at the imaging spectrometer in the aircraft and whose base is the area on the ground that is in the detector's field of view. But as it is here assumed that all the absorbing molecules are in the plume, the column need not extend higher than the top

of plume. Such a column would then be a pyramid with its top clipped off, called a frustum. As the distance from the ground to the top of the plume is assumed to be much shorter than the distance from the top of the plume to the aircraft, this column can be approximated as prism of height  $l$ , where  $l$  is the distance from the ground to the top of the plume. Because we are assuming that the aircraft is directly overhead, the column will be a right prism, rather than an oblique prism. For an aircraft high above the plume, the cross-sectional area of this prism would be approximately constant. This is especially true for the case that we are considering here, an unfilled pixel near the point where it is being discharged into the atmosphere.

The column abundance  $\bar{c}l$  can be expressed in terms of a steady mass flow rate,  $q$ , the wind speed,  $u$ , and the ground sampling distance,  $L$ . For a steady chemical mass flow, the flow into a column extending upwards above the ground and the mass flow out of that column must be equal, not necessarily at every instant, because of atmospheric turbulence, but on average. The equation that specifies that the mass flow into any volume equals the mass flow out of that volume (called the mass balance equation or the equation of continuity) is particularly simple for a column above an underfilled pixel, such as pixels 1 and 2 in Figure 1, in which the all the gas flows into one side of a prism-shaped column and flows out the opposite side. The mass flow into the column is  $q$ . The mass flow out of that column is  $M(\bar{c}l)uL$ , where  $M$  is the molar mass (molecular weight) of the chemical in the plume. The SI unit for molar mass is kg/mol. Setting the mass flow into the column equal to the mass flow out gives

$$q = M(\bar{c}l)uL \quad (8)$$

where  $L$  is the length of the side of the pixel facing the wind, which is called the ground sampling distance. See Figure 1. The distance between the two sides of the column that are perpendicular to the wind is unspecified in Eq. 8; this distance does not have to be numerically equal to the ground sampling distance, but often is.

Substituting Eqs. 7 and 8 into Eq. 5 gives

$$\Delta\Phi_\lambda = (a\kappa_\lambda q/MuL) \left[ B_\lambda(T_{\text{air}}) - B_\lambda(T_{\text{grnd}}) \right] \quad (\text{optically thin plume}) \quad (9)$$

This equation can be used to estimate the mass flow  $q$  required to produce a desired change in the radiant flux  $\Delta\Phi_\lambda$  on a detector element when the ground radiometric temperature is  $T_{\text{grnd}}$  and the air temperature is  $T_{\text{air}}$ . Equation 9 and all the equations derived from it (Eqs. 10-14) are valid only for an optically thin plume.

Substituting Eq. 6 into Eq. 9 gives

$$|\Delta\Phi_\lambda| = (a\kappa_\lambda q/MuL) \frac{\partial B_\lambda}{\partial T} \Delta T \quad (10)$$

The blackbody spectral radiance  $B_\lambda(T)$  and its derivative  $\partial B_\lambda/\partial T$  are functions only of temperature  $T$  and wavelength  $\lambda$ . However, if we approximate  $\partial B_\lambda/\partial T$  as a temperature-independent constant, Eq. 10 can be written as

$$|\Delta\Phi_\lambda| = k_\lambda \kappa_\lambda (q/MuL) \Delta T \quad k_\lambda = a(\partial B_\lambda/\partial T) = \text{temperature-independent constant} \quad (11)$$

We will now show that Eq. 1 can be derived from Eq. 11; consequently, Eq. 1 will be valid under the conditions that Eq. 11 is valid.

Suppose we have determined, by measurement or calculation, that when  $u = u_0$ ,  $L = L_0$ , and  $\Delta T = \Delta T_0$  that  $q_0$  is the minimum mass flow that can be detected. The corresponding change in the radiant flux at wavelength  $\lambda$  would be  $|\Delta\Phi_{\lambda,0}|$ , which would be the minimum detectable change in radiant flux. If we assume these values of  $|\Delta\Phi_{\lambda,0}|$ ,  $q_0$ ,  $u_0$ ,  $L_0$ , and  $\Delta T_0$  satisfy Eq. 11, we have

$$|\Delta\Phi_{\lambda,0}| = k_\lambda \kappa_\lambda (q_0 / M u_0 L_0) \Delta T_0 \quad (12)$$

As pointed out above, this equation is valid for any wavelength for which  $\kappa_\lambda > 0$ . As implied by Eq. 11,  $|\Delta\Phi_{\lambda,0}|$  depends only on the value of  $(q/uL)\Delta T$  and the values of  $k_\lambda$ ,  $\kappa_\lambda$ , and  $M$ , which do not depend on the values of  $q$ ,  $u$ ,  $L$ , or  $\Delta T$ . [Actually,  $\kappa_\lambda$  can be a function of temperature, but only to an insignificant extent.] Consequently, for any measured values of  $u$ ,  $L$ , and  $\Delta T$ , it is possible to find a value for  $q$  (that is, a value for the mass flow rate) such that

$$(q/uL)\Delta T = (q_0/u_0L_0)\Delta T_0 = |\Delta\Phi_{\lambda,0}| / (k_\lambda \kappa_\lambda / M) \quad (13)$$

Solving Eq. 13 for  $q$  gives

$$q = q_0 (u/u_0) (\Delta T_0 / \Delta T) (L/L_0) \quad (14)$$

Equation 14 gives the mass flow rate that will produce the same change in radiant flux on a detector as was produced by mass flow  $q_0$  when  $u = u_0$ ,  $L = L_0$ , and  $\Delta T = \Delta T_0$ . Equation 14 is valid for all wavelengths in the recorded spectrum, provided the plume is optically thin at these wavelengths. Equation 14 does not contain any wavelength-dependent constants, even though it was derived from equations containing the wavelength-dependent constants  $k_\lambda$  and  $\kappa_\lambda$ . This is in part a consequence of the assumption or approximation made in Eq. 11 that  $\partial B_\lambda / \partial T$  is a function of wavelength alone, not temperature. This approximation is examined in Section 2.2.

Equation 1 follows immediately from Eq. 14. Equation 14 gives the mass flow  $q$  that is barely detectable. Equation 1 gives a mass flow that is  $S$  times the mass flow that is barely detectable, that is,  $S$  times the so-called minimum detectable quantity.

In this discussion,  $q_0$  was specified as the minimum detectable quantity. The equations in which  $q_0$  appears would also be valid if  $q_0$  had been specified differently, for example, if  $q_0$  were specified to be the minimum mass flow that could be detected with a high confidence when  $u = u_0$ ,  $L = L_0$ ,  $\Delta T = \Delta T_0$ . For such a specification,  $q$  in Eq. 14 would be minimum mass flow rate that could be detected with a high confidence when the wind speed is  $u$ , the ground sampling distance is  $L$ , and  $|T_{\text{air}} - T_{\text{gnd}}|$  is  $\Delta T$ .

## 2.2 Accuracy

Equation 9 should be accurate if the conditions under which it is derived are met. These conditions include (1) an underfilled pixel placed relative to the wind direction, as shown in Figure 1, (2) the ground radiometric temperature,  $T_{\text{gnd}}$ , everywhere the same within that pixel, (3) an optically thin plume, and (4) absorption by atmospheric gases can be ignored or otherwise accounted for.

Equation 1 is derived from Eq. 9 and the approximations given by Eqs. 6 and 11. So, the accuracy of Eq. 1 depends on the accuracy of Eqs. 6 and 11.

Equation 6 implies that higher order terms in the Taylor expansion are negligible, and Equation 11 implies that  $\partial B_\lambda/\partial T$  is temperature independent. Both are true when  $B_\lambda(T)$  is a linear function of temperature, that is, when

$$B_\lambda(T) = b + mT \quad (\text{condition for Eqs. 6 and 11 to be precisely accurate}) \quad (15)$$

where  $b$  and  $m$  are constants.

As is shown in the graph of Figure 2 and discussed in its legend,  $B_\lambda(T)$  is close to being a linear function of  $T$  in 8–14  $\mu\text{m}$  atmospheric window.

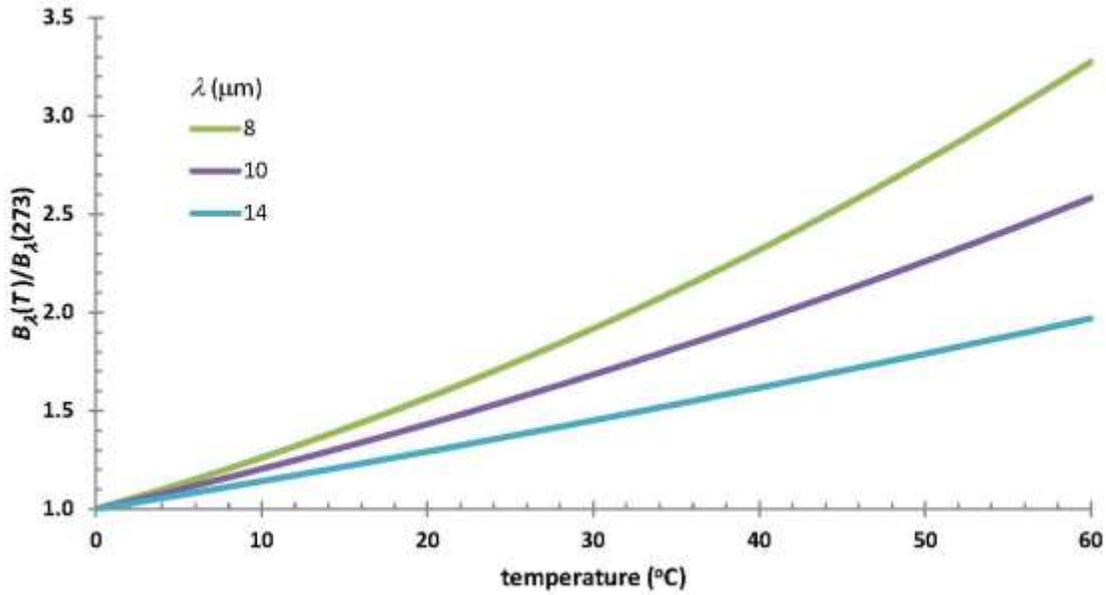


Figure 2. This graph implies that the mathematical approximations used in deriving the equation for sizing chemical flow rates (Eq.1) are acceptably accurate in the long-wave atmospheric window. As discussed in the text, the mathematical approximations in Eqs. 6 and 11 are without error when the blackbody spectral radiance  $B_\lambda(T)$  is a linear function of temperature  $T$ , i.e., a plot of  $B_\lambda(T)$  or  $B_\lambda(T)/B_\lambda(273)$  vs.  $T$  is a straight line.  $B_\lambda(T)$  is the spectral radiance of a blackbody at absolute temperature  $T$ .  $B_\lambda(273)$  is the spectral radiance at  $T = 273.15$  K or  $0^\circ\text{C}$ . Here  $B_\lambda(T)/B_\lambda(273)$  is plotted vs.  $T$  for  $\lambda = 8, 10,$  and  $14 \mu\text{m}$ . Each of these curves is almost a straight line over any  $20^\circ\text{C}$  interval; for example, a straight line extrapolation of  $B_\lambda$  from  $20^\circ\text{C}$  to  $40^\circ\text{C}$  gives a value of  $B_\lambda$  at  $40^\circ\text{C}$  that is 2% too small for  $\lambda = 14 \mu\text{m}$ , 8% too small for  $\lambda = 10 \mu\text{m}$ , and 13% too small for  $\lambda = 8 \mu\text{m}$ .

Even though we measure the wind speed and the ground and air temperatures accurately before the start of a chemical release, we can't, of course, predict exactly what the wind speed and the air and ground temperatures will be at the moment the spectrometer is overhead, imaging the plume. The error in predicting the wind speed can be especially high inasmuch as the instantaneous wind speed can easily vary by a factor of 2 from one minute to the next. Inaccuracies in predicting  $u$  will usually be greater than the inaccuracy of mathematical approximations of Eqs. 6 and 11 in the 8–14  $\mu\text{m}$  atmospheric window. Also, as mentioned above, our ground radiometric temperatures  $T_{\text{grnd}}$  are averages over some wavelength range, e.g., 8-14  $\mu\text{m}$ ; the true ground radiometric temperature at any wavelength in that region is likely to be at least somewhat different from this average. These limitations in determining  $u$ ,  $T_{\text{air}}$ , and  $T_{\text{grnd}}$  rule

against seeking a replacement for Eq. 1 that avoids the mathematical approximations made in its derivation, especially as Eq. 1 is based on an idealized model of underfilled pixels.

Figure 3 shows that in the 3.4–5.0  $\mu\text{m}$  atmospheric window,  $B_\lambda(T)$  is not as close to being the linear function of temperature that it is in the 8–14  $\mu\text{m}$  atmospheric window. Perhaps, the mathematical inaccuracy in Eqs. 6 and 11 will result in chemical release rates that are somewhat higher or lower than desired.

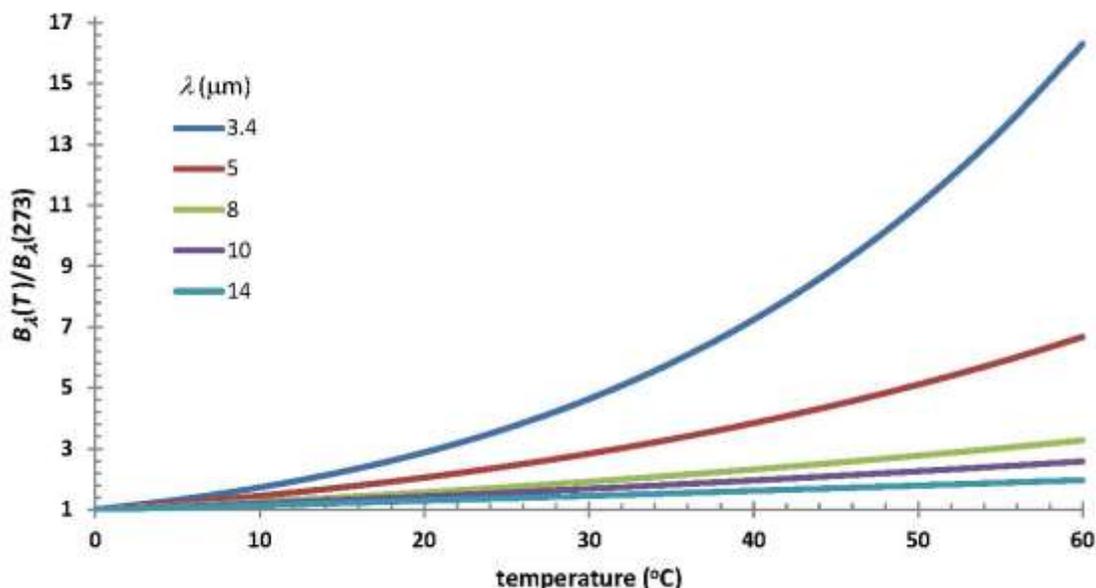


Figure 3. This graph implies that the mathematical approximations used in deriving Eq.1 are less accurate in the mid-wave atmospheric window than in the long-wave atmospheric window. The symbols in this graph have the same meaning as those in the graph of Figure 2. As pointed out in the caption of Figure 2, and as discussed in the text,  $B_\lambda(T)/B_\lambda(273)$  vs.  $T$  must be approximately a straight line for Eq.1 to be approximately accurate. The curves for  $\lambda = 8, 10,$  and  $14 \mu\text{m}$  are the same as those shown in Figure 2, but on a different scale. They are approximately straight lines. The curves for  $\lambda = 3.4$  and  $5.0 \mu\text{m}$  deviate substantially from being a straight line, and so the mathematical approximations on which Eq.1 is based are not particularly accurate. For example, a straight line extrapolation of  $B_\lambda$  from  $20^\circ\text{C}$  to  $40^\circ\text{C}$  gives a value of  $B_\lambda$  at  $40^\circ\text{C}$  that is 23% too small for  $\lambda = 5 \mu\text{m}$  and 35% too small for  $\lambda = 3.4 \mu\text{m}$ . Moreover, the daytime radiometric temperature of a surface at  $3.4 \mu\text{m}$  and at  $4.2 \mu\text{m}$  could be significantly different from the average determined by a  $3.4\text{--}4.2 \mu\text{m}$  radiometer, as solar irradiance is negligible at  $4.2 \mu\text{m}$ , while at  $3.4 \mu\text{m}$ , it can be significant. It could be that Equation 1 should be modified in the  $3.4$  to  $4.2 \mu\text{m}$  region, but we have not investigated that.

Equation 1 should be used only to size chemical flow rates. Tratt et al. [2] summarized the procedures to quantitatively determine chemical mass flow rates from spectra recorded by an airborne infrared imaging spectrometer. Figure 4 is a redraw of Figure 3 in that paper. It shows the accuracy to which methane release rates can be determined from spectra between  $7.6$  and  $8.2 \mu\text{m}$ , a wavelength band at the edge of the atmospheric window where there is interfering water vapor absorption that must be taken into account. The computed flow rates in Fig. 4 used ground measurements of the wind speed and air temperature, as airborne estimations are less accurate.

Figure 4 indirectly shows the accuracy of Eq. 1. We were asked to release methane at a barely detectable level, and released methane at a rate of  $2.2 \text{ kg/h}$ , computing this value using Eq. 1. The methane plume was barely detectable, as shown in Fig 2a in Tratt et al. [2]. This is typical: use of Eq.1 usually results in

flow rates that are near the minimum detectable rate or some specified multiple of it, but seldom precisely so.

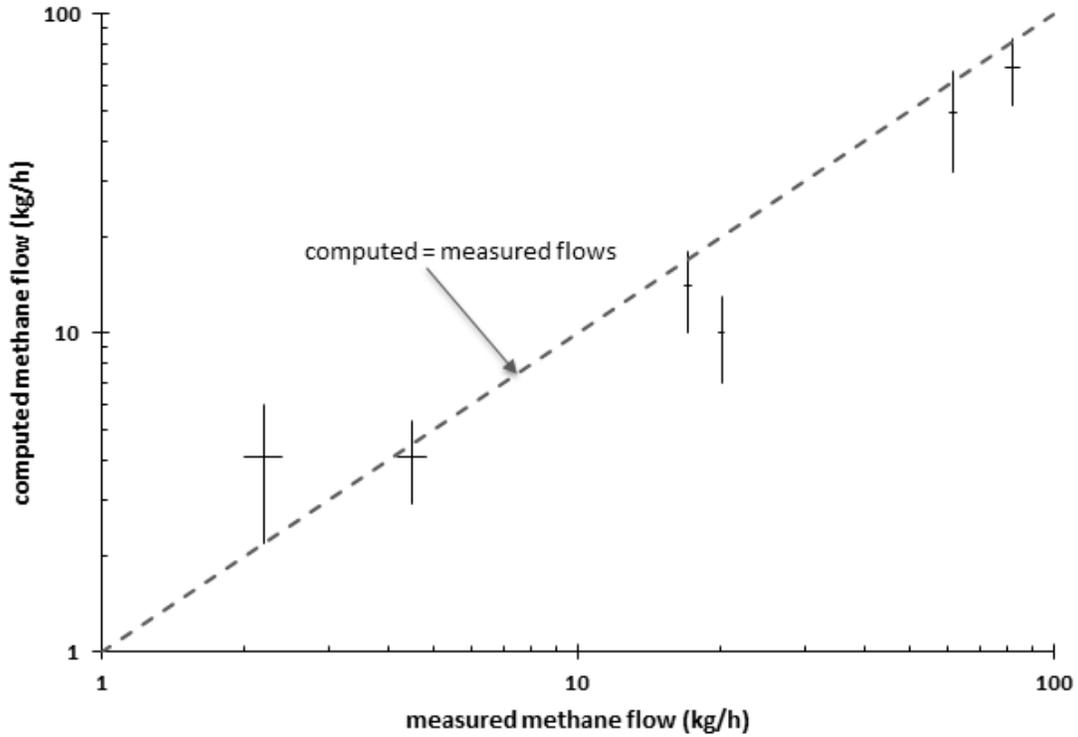


Figure 4. This graph shows the accuracy to which chemical flow rates can be determined from airborne spectra of their downwind plumes. Spectra of methane plumes were taken by The Aerospace Corporation's Mako infrared hyperspectral imaging spectrometer, mounted in a DHC-6 Twin Otter airplane, viewing plumes while directly overhead. The horizontal error bars in this graph give the uncertainties in the measured methane flow rates; the vertical error bars give the uncertainties in methane flow rates computed from the infrared spectra taken by Mako and from ground measurements of wind speed and air temperature. The methane release rates were sized using Eq. 1 and gave the desired flow rates; in particular, the 2.2 kg/h flow rate was sized to be barely detectable, which it was.

### 3. References

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