

E-CALC DESCRIPTION

MINNICH AND SCOTTO, INC.

Rev. February 27, 2018

Minnich and Scotto, Inc. (www.msiair.net) is the architect of e-Calc[®] – an emissions-cal calculation software package developed initially for use with open-path Fourier-transform infrared (FTIR) spectroscopy in order to generate air pollutant emission rates from a wide range of ground-level sources. The software, however, is equally applicable for use with a tunable diode laser (TDL) system, or any other optical remote sensing (ORS) instrument which generates a path-integrated concentration (PIC). It can also be used with a rapid sampling point monitoring device, such as a cavity ring-down spectroscopy (CRDS) system, from which a path-averaged concentration output is derived.

What Are the Benefits of Open-Path Monitoring for Calculating an Emission Rate?

The difference between a source emission rate (mass per time) and an ambient air concentration (mass per volume) is often poorly understood. Further, few investigators appreciate the full utility of the path-integrated concentration when coupled with onsite meteorology and air dispersion modeling for deriving emission rates. When properly applied, an open-path ORS instrument eliminates the spatial data-representativeness problem inherent in emission approaches which rely solely on point-sampling techniques. This path-integrated “whole-plume” measurement approach offers perhaps the only means of fully employing the U.S. EPA’s data quality objective process for generating emission rates, thereby ensuring that end-user needs are always met.

Point-type monitors typically report gaseous concentrations as the mass of contaminant per volume of air, such as milligrams per cubic meter (mg/m^3), or the volume of contaminant per volume of air, such as parts per million (ppmv). Although path-integrated concentrations are often reported as parts-per-million times meter (ppm-m), it is often desirable to convert from ppm-m to milligrams per square meter ($\text{mg}/\text{m}^3 \times \text{m}$, or mg/m^2) in order to avoid having to consider the compound’s molecular weight explicitly in calculating emission rates.

Emission rates derived from point monitoring data are frequently underestimated, as there is no way of knowing the proximity of a hand-held monitor (or Summa canister) to the plume centerline, especially given the fact that wind direction is never constant; in fact, it is generally not possible to ensure that the sample isn’t inadvertently collected completely outside the downwind plume. This fundamental sampling design flaw explains, at least in part, the wide variability in reported emission factors for the same process components (particularly in the oil and gas industry).

Figure 1 illustrates how the pollutant concentration at a location downwind of a small source drops off rapidly as one moves away from the plume centerline.

FIGURE 1. POLLUTANT CONCENTRATION DROP-OFF AWAY FROM THE PLUME CENTERLINE

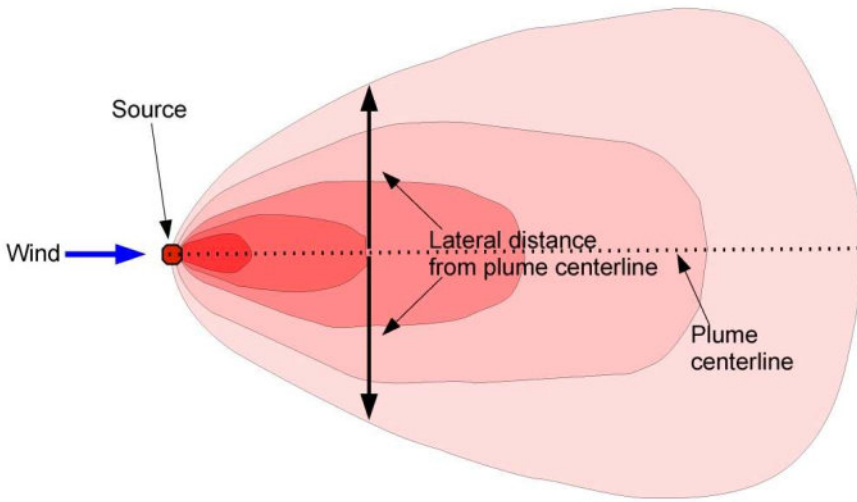
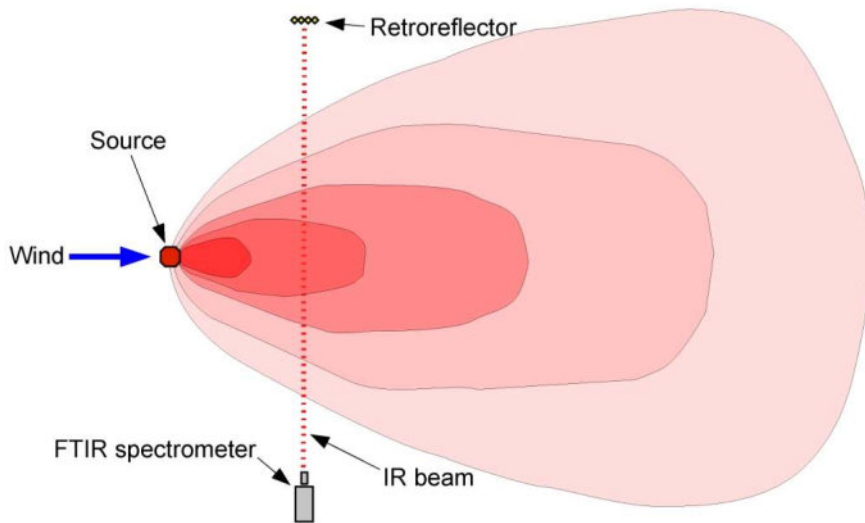


Figure 2 illustrates how the entire crosswind plume is sampled using open-path FTIR spectroscopy (or any other ORS system). The spectrometer collects path-integrated concentration data, meaning that contaminant concentrations are measured downwind of the source along the entire crosswind dimension of the plume. The spectrometer, in essence, counts the molecules of each pollutant, thus ensuring that concentrations are not “missed” anywhere along the beam path (which, for a TDL system, can extend up to a kilometer or more, depending on the application).

FIGURE 2. CROSSWIND PLUME SAMPLING



Open-path spectroscopy is identical to laboratory spectroscopy, except that the “sample” is measured in the open atmosphere rather than from a cell. Because analyses are performed *in situ* (i.e., there is no sample *per se*), all “sample handling” errors are eliminated (another source of negative bias), and re-analysis can be performed at any time in the future – *even for compounds not monitored for originally*.

Using dispersion modeling relationships, a source emission rate is “back-calculated” for a given pollutant based on the downwind (cross-plume) path-integrated concentration and the onsite meteorology representative of the precise monitoring event duration (sometimes referred to as “inverse” modeling).

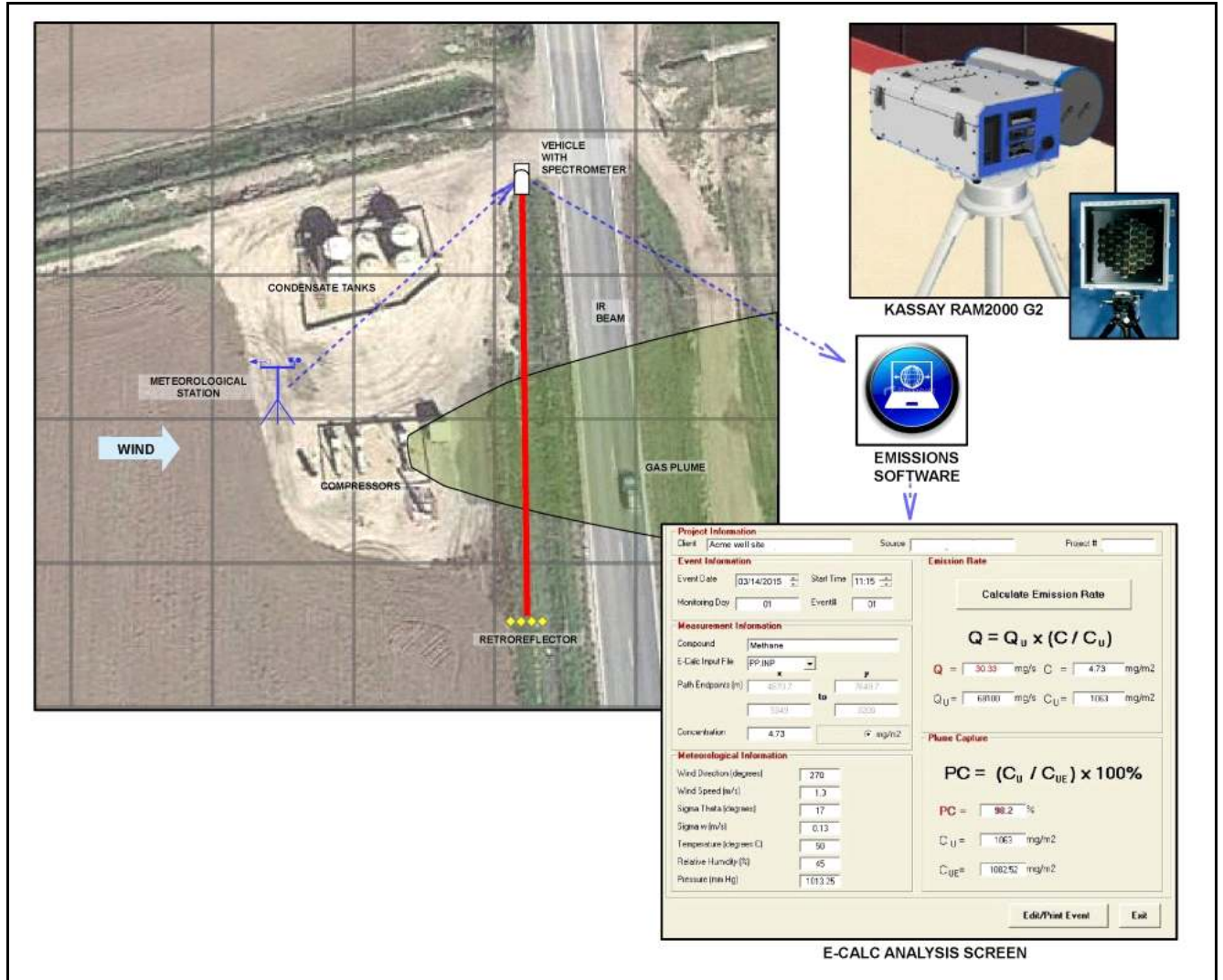
What Exactly is e-Calc?

E-Calc is MSI’s proprietary, Windows-based client-server software for calculating, in real time, contaminant emission rates – precise 15-minute-averaged snapshots – from individual ground-based (or near-ground-based) sources. Originally created for use with open-path FTIR spectroscopy to help municipal solid waste landfill owners comply with mandated emissions reporting and permitting requirements for methane and other greenhouse gases, e-Calc is designed for easy use with any open-path spectrometer. As mentioned earlier, it can even be configured for “path-averaged” concentration data using a point-type monitor. The software is based on AERMOD (American Meteorological Society / EPA Regulatory Model) – the U.S. EPA’s Guideline air dispersion model for regulatory application. It incorporates path-integrated output from the spectrometer with coincident onsite meteorological data and other information.

E-Calc employs the U.S. EPA regulatory version of AERMOD in order to maintain the model’s legal Guideline status. For each monitoring event, generation of input files requires meteorological data together with emissions-characterization and monitoring configuration data. E-Calc currently assigns dispersion coefficients based on wind speed, land use, solar insolation, and statistical data treatments such as the standard deviations of the horizontal wind direction and vertical wind speed.

Figure 3 illustrates the e-Calc measurement system. Most input data is directly measured and entered into the software program automatically. Pre-identified source locations together with beam-path coordinates are manually entered into simple data input screens (not shown). The e-Calc analysis screen is utilized for entry of event-specific meteorological data leading to emissions calculations via AERMOD, as well as the subsequent generation of a hard-copy report for each monitoring event (discussed below).

FIGURE 3. E-CALC MEASUREMENT SYSTEM



How Does e-Calc Work?

Figure 4 depicts the functional logic for e-Calc.

Measured data consist of:

- the 15-minute-averaged open-path concentration data downwind of the source; and
- the onsite meteorology collected from the portable tower, as well as other parameters such as solar elevation angle and temperature.

Simulated data include:

- boundary-layer data which is pre-processed by AERMET;
- surface characterization information from the NLCD (National Land Cover Data) database and pre-processed by AERSFC; and
- source and beam path location using site plans and USGS coordinate imagery.

FIGURE 4. E-CALC FUNCTIONAL LOGIC

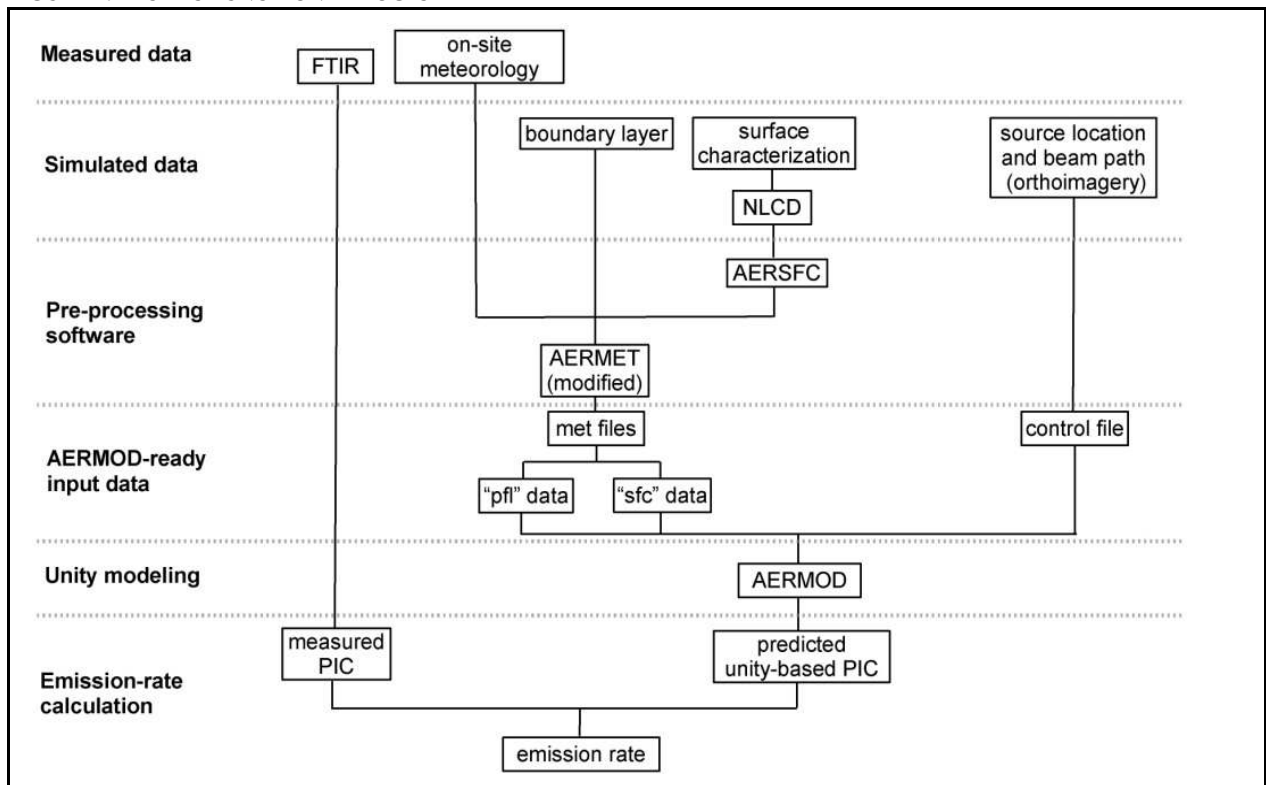


Figure 5 presents an example e-Calc analysis screen. The AERMOD output file includes all input data, a model set-up summary, and unity-modeling results for each 15-minute monitoring event.

FIGURE 5. E-CALC ANALYSIS SCREEN

Project Information
 Client: ACME Gas Company Source: Condensate Tank Hatch Project #: 547.03

Event Information
 Event Date: 09/14/2015 Start Time: 08:00
 Monitoring Day: 01 Event#: 01

Measurement Information
 Compound: Methane
 E-Calc Input File: W03.INP
 Path Endpoints (m): 1025 to 975
 Concentration: 1.7 mg/m²

Meteorological Information
 Wind Direction (degrees): 245
 Wind Speed (m/s): 1.81
 Sigma Theta (degrees): 10.26
 Sigma w (m/s) (9999 if missing): 0.17
 Temperature (degrees C): 13.9
 Solar Elevation Angle: 12.4
 Cloud Cover (0-10): 0
 Relative Humidity (%): 37
 Pressure (mm Hg): 1013.25

Emission Rate
 Calculate Emission Rate
 $Q = Q_U \times (C / C_U)$
 Q = 29 mg/s C = 1.7 mg/m²
 Q_U = 314.16 mg/s C_U = 18.42 mg/m²

Plume Capture
 $PC = (C_U / C_{UE}) \times 100\%$
 PC = 97.1 %
 C_U = 18.42 mg/m²
 C_{UE} = 18.96 mg/m²

Edit/Print Event Exit

How Exactly Are Emissions Derived?

Emission rates of each target compound (pollutant) are calculated in accordance with the *area-source technique*, in which the following relationship holds:

$$C / Q = C_U / Q_U \quad \text{(Equation 1)}$$

where:

- C = measured path-integrated concentration (attribution) (mg/m²);
- Q = actual emission rate (mg/s);
- C_U = predicted unity-based path-integrated concentration along the measurement path (mg/m²); and
- Q_U = unity-based emission rate (mg/s).

Equation 1 describes the inherent relationship between: (a) the unity-based dispersion modeling; and (b) the actual emission rate and downwind measurements. The cornerstone of the *area-source technique*, this ratio states that the measured path-integrated concentration is to the actual emission rate as the unity-based path-integrated (modeled) concentration is to *its* unity-based emission rate. The only unknown term in this equation is the actual emission rate (Q).

The spectrometer generates the measured path-integrated concentration (C). AERMOD is configured to yield a predicted concentration for each meter along the beam path; these predictions are summed to derive the predicted unity-based path-integrated concentration (C_U).

Assignment of the unity-based emission rate (Q_U) is straightforward (i.e., simply set to 1 mg/s), unless the source includes multiple emission “subareas” of varying magnitude; in such a case, multiples of unity are assigned to each subarea based either on determination of *relative source strengths* or on best professional judgement.

What Does an e-Calc Monitoring Event Report Look Like?

Figure 6 presents an actual e-Calc monitoring event report for a large (1 square kilometer) process pond in support of an Alabama paper mill, against which a nuisance lawsuit was brought by the nearby community.

FIGURE 6. E-CALC MONITORING EVENT REPORT

E-CALC MONITORING EVENT REPORT	
EVENT SUMMARY	
EVENT # (E-__)	7
SOURCE	Polishing Pond
HYDROGEN SULFIDE EMISSION RATE	9.6 lb/hr
PLUME CAPTURE	77.5 %

Project Information	Event Information
CLIENT International Paper	EVENT # (E-__)
SOURCE Polishing Pond	MONITORING DAY 2
PROJECT # 538.01	DATE 06/30/2011
	START TIME 11:00
	E-CALC INPUT FILE P12-0207
Meteorological Information	Emissions Information
WIND DIRECTION 340.1 degrees	Q = Q_U x (C / C_U)
WIND SPEED 2.643 m/s	EMISSION RATE (Q) 1,207.7 mg/s 9.6 lb/hr
SIGMA THETA 28.14 degrees	UNITY EMISSION RATE (Q _U) 68,772.49 mg/s
SIGMA W 0.242 m/s	CONCENTRATION (C) 30.3 mg/m ²
TEMPERATURE 32.2 degrees C	UNITY CONCENTRATION (C _U) 1,725.41 mg/m ²
SOLAR ELEVATION ANGLE 64.99 degrees	
CLOUD COVER 0 tenths	
Plume-Capture Results	
PC = (C_U / C_{UE}) x 100%	
PLUME CAPTURE (PC)	77.5 %
UNITY CONCENTRATION (C _U)	1,725.41 mg/m ²
EXTENDED-PATH UNITY CONCENTRATION (C _{UE})	2,226.80 mg/m ²

Can e-Calc be Used to Assess Community Impacts?

Yes. An e-Calc-derived source term can be directly input to AERMOD for prediction – via forward modeling – of downwind community impacts across any specified receptor field. MSI will work with customers on an application-specific basis to address such needs.

What Are MSI's Plans to Upgrade E-Calc?

E-Calc is the most sophisticated software on the market today for generating emission rates from area-type sources directly from open-path measurements and onsite meteorological data. Nonetheless, MSI has consulted with AERMOD developers to optimize treatment of the dispersion and transport component in order to maximize e-Calc accuracy; this optimization process is dynamic as some of the effort draws upon results of ongoing field work. MSI also intends to expand e-Calc to include treatment of additional source types.

Following is a description of anticipated upgrades to e-Calc in terms of: (a) the measured data and pre-processing software (to maximize emissions accuracy) as depicted in Figure 4; and (b) additional source types.

Measured Data

The onsite meteorology in the current version of e-Calc is collected largely via a standard cup-and-vane sensor. Wind direction, wind speed, sigma theta or σ_{θ} (standard deviation of the horizontal wind direction), and sigma W or σ_w (standard deviation of the vertical wind speed) are collected (or calculated) from an appropriately configured 3-meter meteorological tower. Air temperature is measured using a portable hand-held instrument, and cloud cover (in tenths) is observed and recorded; the solar elevation angle is calculated in accordance with the National Oceanic and Atmospheric Administration (NOAA) Solar Calculator.

MSI anticipates that an upgraded version of e-Calc will include output from a 3D sonic anemometer and temperature sensor for direct measurement of boundary layer parameters. The sensors measure 1-second orthogonal wind and temperature, from which the 15-minute-averaged covariance is generated between the u and w wind components, the v and w wind components, and the w wind component and temperature. (Note: this improvement is consistent with changes the U.S. EPA currently anticipates for AERMOD but has not yet implemented; accordingly, this e-Calc upgrade should prove invaluable in support of ongoing AERMOD research.)

Pre-Processing Software

Boundary layer parameters (e.g., friction velocity, sensible heat flux, Monin-Obukhov length) are required in the surface data meteorological file input to AERMOD. In the current version of e-Calc, these boundary layer parameters are simulated indirectly based on the *flux-gradient approach* employed in the AERMET preprocessor (shown in Figure 4); use of this approach is necessitated by the type of meteorological data collected via the cup-and-vane wind sensor.

The upgraded version of e-Calc will likely include an option for the direct measurement of boundary layer parameters using the *eddy-correlation (or covariance) approach*, thus obviating the need for the AERMET preprocessor. In this approach, both the friction velocity and the Monin-Obukhov length are calculated using the covariance statistic between the u and w wind components and the v and w wind components; sensible heat flux is calculated using the covariance between the w wind component and temperature.

Additional Source Types

The upgraded version will include an option for modeling volume sources (e.g., natural gas gathering pipeline assemblies having multiple small flange and valve leaks) and near-ground stack- and vent-type sources (e.g., condensate tank vents).

How Can ORS Address the Monitoring Needs of a Complex Source Such as a Refinery?

For a petrochemical refinery or other large complex source (or groups of sources), there are any number of air-related needs or objectives that open-path UV DOAS or FTIR spectroscopy can play an integral role in achieving, depending on the pollutants of concern and the proximity of the source(s) to the local residents. These include:

- Emission-rate quantitation on a total facility basis in order to assess compliance with applicable emission standards for criteria pollutants, HAP (Hazardous Air Pollutants), or greenhouse gases;
- Emission-rate quantitation on a process-unit basis in order to assess compliance with NSPS (New Source Performance Standards), NESHAP (National Emissions Standards for HAP), or MACT (Maximum Available Control Technology);
- Emissions inventory tabulation in order to support permit compliance, TRI (Toxic Release Inventory) reporting, or refinery RTR (Risk and Technology Review);
- Real-time process monitoring in order to identify and facilitate mitigation of emissions associated with start-up, shutdown, and malfunction (SSM) events;
- Compliance with fenceline monitoring requirements pursuant to U.S. EPA's June 2014 proposed Petroleum Refinery Sector Risk rule;
- Demonstration that pre-established time-averaged "safe" levels are not contravened (either at the facility boundary or in the downwind community); and
- Depiction of real-time community HAP exposure to the public in order to facilitate positive public relations.

Regardless of a facility's specific needs, the challenge of addressing simultaneous emissions from multiple sources requires the formulation of a clear understanding of each objective. ***Hence, the notion of a "one-size-fits-all" solution can be dismissed based simply on the number of variables which must be considered.***

As stated earlier, e-Calc itself can handle only individual sources; nonetheless, e-Calc provides the main "building blocks" for development of a **Customized Software Solution** to address each such facility need. In all instances, this process begins with a case-by-case review of available source-specific information and data such as:

- A site plan depicting the facility boundary and locations of those process operations having the potential for generating air pollutant emissions;
- A copy of all facility operating permits (and approved permit application documentation) which detail emissions data by facility or process unit;
- Preliminary source emission-rate estimates based on available U.S. EPA emission factors (e.g., AP-42) and relevant guidance;
- Identification of all compounds (pollutants and otherwise) which may be generated from each process unit and not reported in existing operating permits; and
- Existing air quality data collected from third parties (e.g., the impacted community).

A **Customized Software Solution** will likely require implementation of any or all of the following "tools" to augment e-Calc:

- Controlled Tracer Release
A controlled tracer may be released from a group of sources to confirm the source identification and provide the basis for more accurate simulation of plume dispersion (either via model calibration or employment of an empirical model correction factor).
- Thermal Imaging Camera
In order to address complex source configurations, a thermal imaging camera can be utilized to precisely locate a leaking source as well as provide an objective measure of the *relative source strength* (necessary for use in AERMOD, as discussed previously). "Hot spots" are represented in the unity modeling by assigning these unique source strengths to each source subarea (i.e., leak).

- Measurement Path “Segmenting”
Individual segments comprising the measurement path may be examined under a range of meteorological conditions in order to identify the attribution of a particular source (or combination of sources).

How Does a Customized Software Solution Compare with OTM-10?

U.S. EPA Other Test Method 10 (OTM-10), “Optical Remote Sensing for Emission Characterization from Non-point Sources” (Final ORS Protocol, June 14, 2006), describes three emission methods: horizontal radial plume mapping (HRPM), vertical radial plume mapping (VRPM), and one-dimensional radial plume mapping (1D-RPM). Only the VRPM Method is potentially applicable to address the needs or objectives identified earlier for complex sources.

Per OTM-10 (page 1), the VRPM Method “was designed to measure [the] mass flux of pollutants through a vertical plane, downwind from an emission source.” From page 3, the VRPM Method “utilizes multiple non-intersecting beam paths in a vertical plane downwind from the emission source to obtain a mass-equivalent plume map. This map, in conjunction with wind speed and direction, is used to obtain the flux of pollutants through the vertical plane.”

Implementation of the VRPM Method has several serious drawbacks. On a technical basis, the method accuracy is directly proportional to how wind speed and direction varies with height across the vertical (and horizontal) dimensions of the plane, factors which heretofore have been ignored. Secondly, without careful meteorological monitoring and reliance on dispersion modeling (which the method seeks to avoid), the possibility of substantial portions of the plume going above or outside of the vertical plane will always exist (especially under unstable atmospheric conditions or when the distance between the plane and the upwind emission source is relatively large) – thus contributing strongly to the marginal degree of emissions reproducibility at best, and then for only the simplest of controlled ground-level source releases. Finally, since the VRPM Method does not incorporate relative emission strength and location information for individual source subareas, only a crude total facility flux (or emission rate) can ever be ascertained.

On cost and logistical bases, unless multiple vertical planes are erected around a source (which will generally be prohibitively expensive), long periods of time will frequently elapse before a suitable combination of wind direction and stability will occur.

Conversely, for either e-Calc or any **Customized Software Solution**, there is never a need to directly consider pollutant concentrations or meteorology in the vertical dimension, as a precise measure of atmospheric dispersion coefficients (given via detailed assessment of atmospheric turbulence) allows for the three-dimensional behavior of the contaminant plume to be accurately determined based on mass-balance considerations inherent in AERMOD. E-Calc has an added feature which calculates the mass of the plume capture (as a percentage) based on the measurement path distance and orientation, and automatically adjusts the emission rate accordingly.

Further, as system set-up can be accomplished in about an hour, the only constraints will generally be line-of-sight. Finally, the cost to implement a **Customized Software Solution** will generally range between 50 and 90 percent *less* than the VRPM Method.

* * * * *