Real-Time Detection of Ethylene Oxide in Ambient Air with Limited Interferences

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Introduction

Ethylene oxide is an emerging contaminant of increasing interest to regulatory agencies. Commonly used, real-time, direct mass-spectrometric methods – specifically, proton-transfer-reaction (PTR) – face severe limitations in monitoring ethylene oxide in ambient air due to interferences. Ethylene oxide with typical background concentration of hundreds of part-per-trillion (ppt) shares the same protonated mass-to-charge ratio as acetaldehyde (45 Th, $C_2H_4O{\bullet}H^+$), which is ubiquitous in the atmosphere at typically much higher background concentrations.

Ethylene Oxide Detection with the Vocus CI-TOF

The following method using the Vocus CI-TOF mass spectrometer equipped with the Vocus PTR Reactor allows sensitive, real-time measurement of ethylene oxide in ambient air without interference from acetaldehyde. This method can be additionally used for the detection of aromatics (e.g. BTX) and terpenes. It uses ultra-high purity (UHP) oxygen (O_2) as a reagent gas to generate O_2^+ reagent ions. The target analytes can undergo ionization through three distinct pathways including charge transfer for aromatic compounds (BTX), hydride abstraction for aldehydes (propanal, acetaldehyde), and adduct formation for ethylene oxide.

Results

In Figure 1 two overlaying mass spectra of two separate measurements of ethylene oxide and acetaldehyde, both at mixing ratio of 20 parts per billion (ppb), are presented. The figure illustrates the distinct detection of ethylene oxide as a cluster $C_2H_4O{\bullet}O_2^+$ at mass-to-charge ratio 76. Additionally, it highlights the minimal interference from acetaldehyde, which is less than 0.5%. Acetaldehyde can be detected as $C_2H_3O^+$ at mass-to-charge ratio 43 Th.

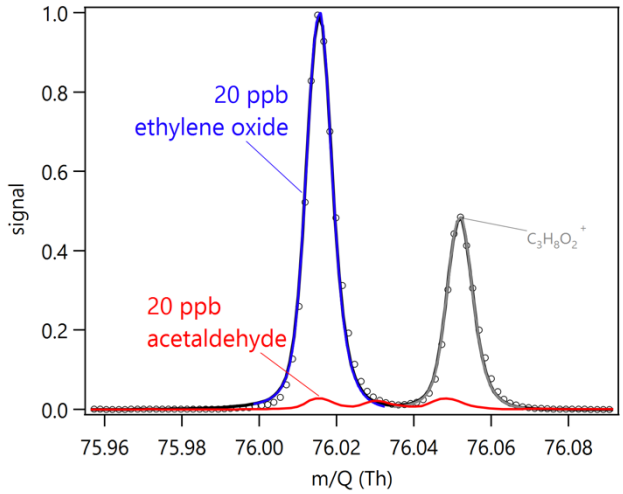

Figure 1. *Normalized signal for measurement of ethylene oxide, without acetaldehyde, is shown in blue. Normalized signal for measurement of acetaldehyde, with no ethylene oxide, is shown in red.*

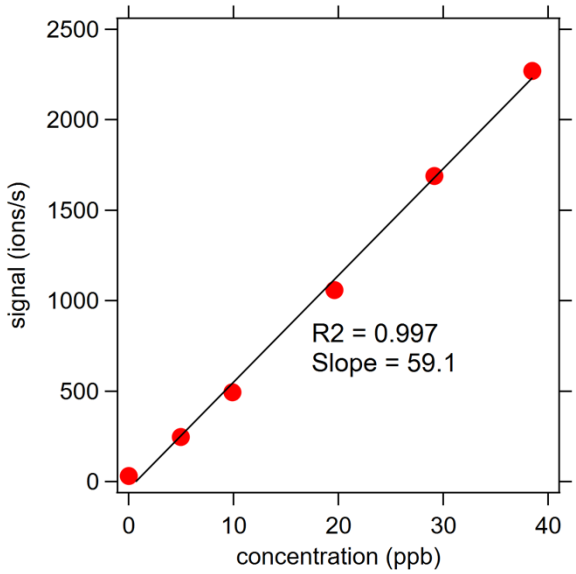

Figure 2*. Calibration curve for ethylene oxide.*

Results

In Figure 2 a six-point calibration curve relating the concentration of ethylene oxide to the measured signal is shown. The curve demonstrates that the analytical method exhibits a linear response while the slope indicates the sensitivity which is equal to 59 counts per second (cps) per ppb.

In Table 1, calculated limits of detection (LODs), defined as three times standard deviation of signal in clean air, for ethylene oxide and other selected species are reported. The LODs were directly measured

Compound	Detected as	2R/S		Scout		Eiger	
		1-sec.	*1-min.*	*1-sec.*	*1-min.*	*1-sec.*	*1-min.*
		ppt		*ppt*		*ppt*	
Ethylene oxide	$C_2H_4O{\bullet}O_2^+$	270	29	400	40	850	90
Benzene	$C_6H_6^+$	14	1.0	20	2	40	3
Toluene	$C_7H_8^+$	11	0.80	15	1	40	3
Xylene	$C_8H_{10}^+$	15	1.2	20	2	40	4
Trimethylbenzene	$C_9H_{12}^+$	19	1.9	30	3	60	6
Propanal	$C_3H_5O^+$	150	13	250	20	500	40
α-pinene	$C_{10}H_{16}^+$	100	11	150	15	350	30

Table 1. *Limits of detection for selected volatile organic compounds reported. The LODs were calculated for 1-second and 1-minute integration times.*

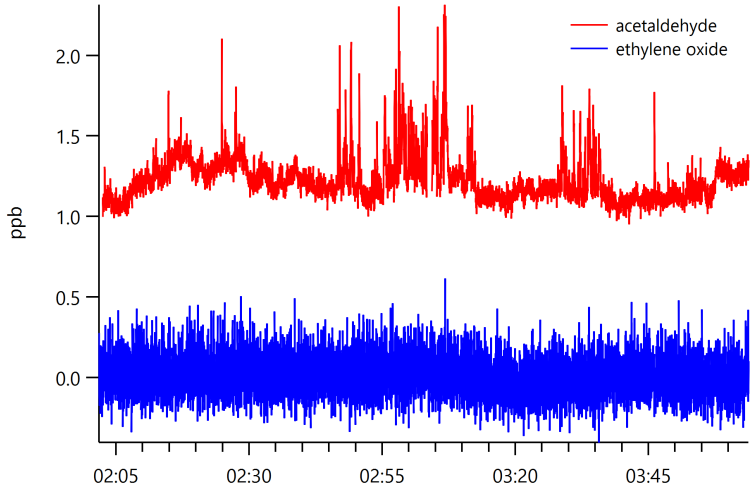

Figure 3. *Time series of acetaldehyde and ethylene oxide measured in urban ambient atmosphere*

using a Vocus 2R model. The LODs for other models present in the table were derived using typical relative sensitivities for such models.

Figure 3 illustrates real-time simultaneous measurement of acetaldehyde and ethylene oxide in ambient urban air. As anticipated, acetaldehyde exhibits elevated mixing ratios and frequent spike events in the measurements, reflecting its relatively higher prevalence in the atmosphere. On contrary, ethylene oxide, which is scarcer on atmospheric sources, maintains a steady background level. The distinct time evolution provides further evidence of the possibility of differentiation these two species within one measured dataset.

Summary

The analytical method described in this application note can be valuable in various scenarios. Real-time measurement of ethylene oxide is essential for ensuring workplace safety in industrial settings, in environmental stationary or mobile monitoring evaluating potential contamination or compliance with air standards. Further, this technique can be used in emergency response, providing rapid, on-site detection of ethylene oxide during chemical spills. It is also well suited for product quality control where headspace sample analysis serves as verification that the product underwent ethylene oxide treatment such as for medical devices, pharmaceuticals, or personal care products.

Recommended Vocus Models for Ethylene Oxide Detection

This method is compatible with Vocus CI-TOF Eiger, Scout, S, and 2R models, when utilizing the Vocus PTR Reactor. Instruments already equipped with selective reagent ion option (O_2^+ and/or NO^+) can use this method without requiring any hardware alterations. Instruments only capable of H_3O^+ ion chemistry may use this method with minor hardware modifications. The only additional consumable required is UHP oxygen. The Vocus Elf model is not recommended for this measurement due to its unit mass resolving power which does not permit the separation of ethylene oxide from an isobaric interference in ambient air. This model could be used in scenarios where the isobaric interference is insignificant compared to ethylene oxide.

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