

# **SANDIA REPORT**

SAND2004-2117  
Unlimited Release  
Printed May 2004

## **Large-Volume Sampling and Preconcentration for Trace Explosives Detection**

Kevin L. Linker

Prepared by  
Sandia National Laboratories  
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Approved for public release; further dissemination unlimited.



.Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

**NOTICE:** This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from

U.S. Department of Energy  
Office of Scientific and Technical Information  
P.O. Box 62  
Oak Ridge, TN 37831

Telephone: (865)576-8401

Facsimile: (865)576-5728

E-Mail: [reports@adonis.osti.gov](mailto:reports@adonis.osti.gov)

Online ordering: <http://www.doc.gov/bridge>

Available to the public from

U.S. Department of Commerce  
National Technical Information Service  
5285 Port Royal Rd.  
Springfield, VA 22161

Telephone: (800)553-6847

Facsimile: (703)605-6900

E-Mail: [orders@ntis.fedworld.gov](mailto:orders@ntis.fedworld.gov)

Online ordering: <http://www.ntis.gov/ordering.htm>



SAND2004-2117  
Unlimited Release  
Printed May 2004

## **Large-Volume Sampling and Preconcentration for Trace Explosives Detection**

Kevin L. Linker

Entry Control and Contraband Detection Technologies  
Sandia National Laboratories  
PO Box 5800  
Albuquerque, NM 87185-0782

### **Abstract**

A trace explosives detection system typically contains three subsystems: sample collection, preconcentration, and detection. Sample collection of trace explosives (vapor and particulate) through large volumes of airflow helps reduce sampling time while increasing the amount of dilute sample collected. Preconcentration of the collected sample before introduction into the detector improves the sensitivity of the detector because of the increase in sample concentration. By combining large-volume sample collection and preconcentration, an improvement in the detection of explosives is possible. Large-volume sampling and preconcentration is presented using a systems level approach. In addition, the engineering of large-volume sampling and preconcentration for the trace detection of explosives is explained.

# **Acknowledgment**

The author thanks Charles L. Rhykerd, Jr. for his contribution in developing the modeling theory for trace detection systems presented in this document.

# Contents

1. Introduction.....	7
2. Mathematical Model of Trace Detection System .....	8
3. Large-Volume Sample Collection .....	10
4. Preconcentration .....	16
5. Conclusion .....	18
6. References.....	19

## Figures

Figure 1. Mass Sample Distribution in a Trace Detection System.....	9
Figure 2. Local Exhaust System .....	10
Figure 3. Closed and Open Hoods .....	11
Figure 4. Capture and Face Velocities.....	12
Figure 5. Exhausting versus Blowing.....	13
Figure 6. Open Hood with Baffles.....	13
Figure 7. Capture Velocity versus Distance from Hood Face .....	14
Figure 8. Push-Pull Airflows in Sandia Portal.....	15
Figure 9. Large-Volume Preconcentrator Operation .....	16
Figure 10. Sandia Large-Volume Preconcentrators (Inlet sizes: 9-inch, 6-inch, 2-inch) .....	17

## Tables

Table 1. Characteristics of Sandia Preconcentrators .....	17
---	----

## Acronyms

cfm	cubic feet per minute
FAA	Federal Aviation Administration
fpn	feet per minute

# 1. Introduction

Effectively employing trace detection as a method for evaluating the potential presence of explosives requires a systems-level approach on a case-by-case basis. This systems approach should be applied to each technology under consideration for trace detection. Each system should, however, include three subsystems - sample collection, preconcentration, and detection. These subsystems contribute to a trace detection system, as follows.

- **Sample Collection** – Removes and transports sample (vapor and particulate) from a target to the preconcentrator. The method of collection can be invasive, such as swiping, or noninvasive, such as air sampling.
- **Preconcentration** – Concentrates a limited explosives sample. The preconcentrator can take the form of a cotton swab, “swipe,” or a mechanical system.
- **Detection** – Accepts a sample from the preconcentrator and analyzes it. Several types of detection technology are available, such as an ion-mobility spectroscopy, mass spectroscopy, infrared spectroscopy, etc.<sup>1</sup>

Two of these subsystems are often overlooked: sample collection and preconcentration. This lack of attention is due in part to the significant advances that have been made in detector technology and the difficulty in applying sampling and preconcentration technology to low vapor pressure explosives. Despite increased detector sensitivity, sample collection and preconcentration can determine the ultimate success of a trace explosives detection system.

During Sandia’s research and development of a trace explosives detection portal for the Federal Aviation Administration (FAA), much knowledge of sample collection and preconcentration was gained. Sample collection and preconcentration are significant subsystems in the portal because the target to be screened is physically large (the entire human body) and a speedy throughput rate is required (6- to 8- second screening criterion) to accommodate high-volume security screening points such as airports. The portal projects led Sandia to develop large-volume sampling and preconcentration technologies that were subsequently patented and licensed to the commercial sector. In addition to hardware development, a mathematical model to describe and evaluate an entire trace detection system was conceptualized. This model explains the importance of sample collection and preconcentration in a trace system. The large-volume sampling and preconcentration technologies and the mathematical model have been successfully applied to other trace explosives detection systems developed by Sandia, including handheld systems and a prototype vehicle portal.

## 2. Mathematical Model of Trace Detection System

The mathematical model was formulated to support the research and development of sampling and preconcentration technology at Sandia.<sup>2</sup> The model provides the basis for describing trace explosives detection systems and is independent of the specific sampling techniques, preconcentration technology, or detector. Through the model a relative measure of a trace explosives detection system can be determined, which provides a means for comparing trace detection systems for similar applications.

A trace explosives detection system will produce a signal output depending on the concentration of explosives reaching the detector. The following equation shows the relationship of sample collection, preconcentration, and detection in a trace detection system. This equation contains measurable parameters such as:

- initial contamination level;
- sample removal and transport from a target;
- collection of the sample in the preconcentrator, and additional preconcentration, if applicable;
- a term accounting for flow mismatches between the detector inlet and the preconcentrator subsystem outlet; and
- a proportionality term relating signal strength to concentration at the detector.

$$S = M_0 \eta_r \eta_c C_1 \dots C_n (Q_d / Q_n) k \quad [1]$$

where,

$S$  = signal output from the detector

$M_0$  = initial mass of explosives on target (vapor and/or particles)

- **Sample Collection Factors**

$\eta_r$  = fraction of mass on target that is removed from target by sample collection subsystem

$\eta_c$  = fraction of mass removed that is collected in the preconcentration subsystem

- **Preconcentration Factors**

$C_1$  = concentration gain of the 1<sup>st</sup> preconcentration stage

$C_n$  = concentration gain of the n<sup>th</sup> preconcentration stage if applicable, with each preconcentration stage included, 1 to n

- **Detector Factors**

$Q_d$  = inlet (sampling) flow rate of the particular detector

$Q_n$  = output flow rate from the final preconcentration stage

$k$  = proportionality term relating signal strength to concentration at the detector

The efficiencies for sample removal and collection must be between zero and one,  $0 < \eta_r \leq 1.0$  and  $0 < \eta_c \leq 1.0$

Although it appears that  $\eta_c$  is part of the preconcentration term and not sample collection, this is a difference between mathematical modeling and hardware operation. With hardware, sample collection is a function of both the sample collection and preconcentrator. The sample collection subsystem is designed to remove a sample efficiently from the target and transport the sample to



the preconcentrator. The preconcentrator then traps or collects the sample for subsequent detection. Sample collection and preconcentration must be integrated for optimum performance in a trace detection system.

$C_1, \dots$  and  $C_n$  define the preconcentrator performance by combining the efficiencies of adsorption and desorption and the ratio of the volume of flow into each stage during adsorption and out of each stage during desorption.<sup>3</sup> The terms  $C_1, \dots$  and  $C_n$  are further defined as follows.

$$C = \eta_p V_a / V_p \quad [2]$$

where,

$\eta_p$  = preconcentrator efficiency

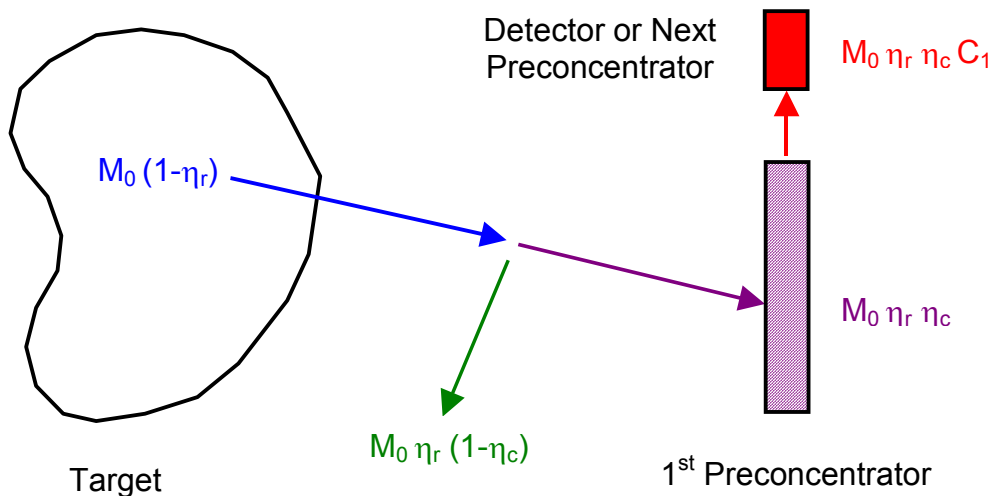
$V_a$  = volume of airflow that passed through the preconcentrator during the adsorption (collection) phase

$V_p$  = internal volume of the preconcentrator or volume into which the explosives sample are desorbed

The preconcentrator efficiency,  $\eta_p$ , accounts for several factors associated with the preconcentrator design. These factors include explosives sample passing through the preconcentrator during the adsorption (collection) phase, explosives sample loss due to adsorption on cool internal surfaces, and molecular decomposition associated with the desorption phase in the preconcentrator.

The value for  $\eta_p$  ranges from 0 (no explosives sample delivered to the detector) to 1 (the entire explosives sample delivered to the detector). Ideally  $\eta_p$  would be 1.

Figure 1 indicates how the initial mass,  $M_0$ , is fractionally distributed through a trace detection system that uses airflow for sample collection.



**Figure 1. Mass Sample Distribution in a Trace Detection System**

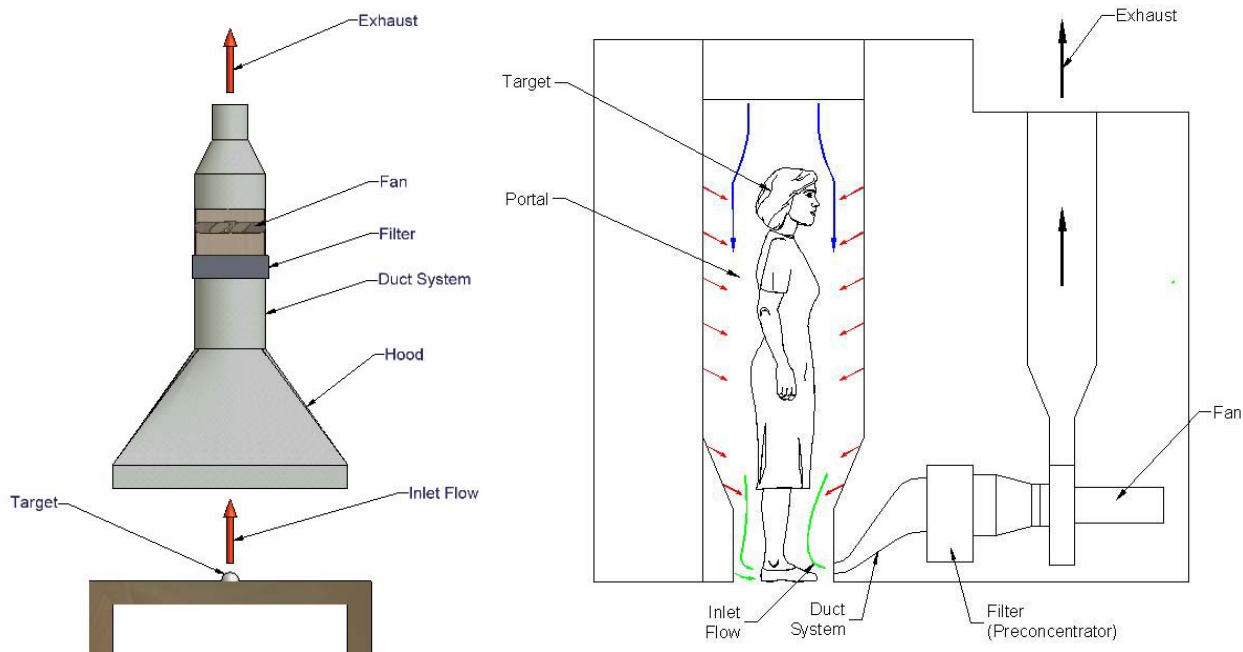
The mathematical model demonstrates the importance of sample collection and preconcentration in a trace detection system. Optimizing the sample removal, transport, collection, and delivery will enhance the performance of the entire trace detection system. Sandia's methodology of non-invasive, large-volume sampling and preconcentration is such an effort at optimization.

### 3. Large-Volume Sample Collection

The collection of a sample in a trace detection system can be compared directly to local exhaust ventilation systems used in industry for contamination control, e.g., welding hoods, open vapor tanks, and fume hoods. Local exhaust ventilation systems operate on the principle of capturing a contaminant (vapors or particles) at or near the source using a fan to induce airflow. In a trace detection system, the contaminant is the explosives sample (vapor or particulate) and the source is the target (human body, baggage, etc.). The local exhaust method is preferred in industrial applications because it is more efficient in contaminant collection and uses less horsepower in the fan.

During Sandia's development of the explosives detection portal, the concept of local exhaust ventilation for sample collection provided the best method for obtaining sample and delivering it to a detector by optimizing  $\eta_r$  and  $\eta_c$  of Equation 1. In addition, this method of sample collection meets the FAA portal design criteria of minimal discomfort to the passenger, reduced impediment to traffic flow (no doors), and a high throughput rate (6 to 8 seconds per passenger).

The similarities of a local exhaust ventilation system and a trace detection system such as Sandia's explosives detection portal are shown in Figure 2. The role of the hood (portal) is to collect the contaminant (explosives sample) by capture and entrainment in an airflow stream and exhaust the contaminant through a filter (preconcentrator). The fan for both provides the airflow through the hood/portal, duct, and filter/preconcentrator.



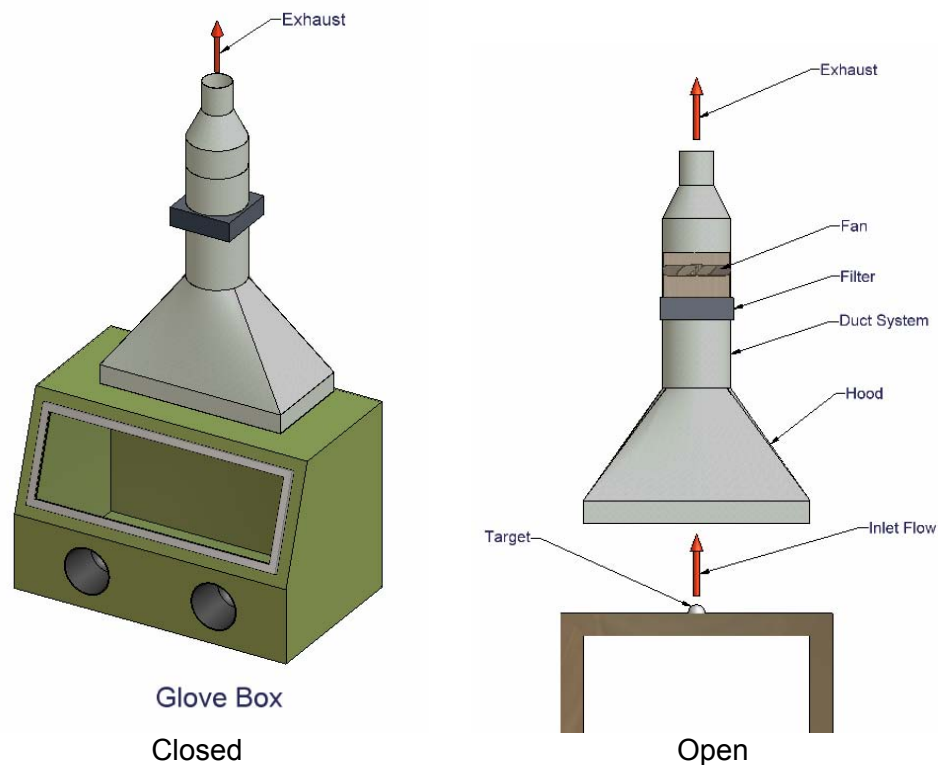
**Figure 2. Local Exhaust System**

Hood designs vary in their physical configurations. The hood configuration will depend on the target and sample to be collected. Hood designs fall into two general categories: closed and open. Closed hoods are those designs that completely or partially enclose the target. Open hoods are located near the target without enclosing. Figure 3 shows examples of the hood categories.

Two factors must be considered when designing a hood.<sup>4,5</sup> First, capturing and transporting a sample will depend on the exhaust flow into the hood. Second, the airflow toward the hood opening must be sufficient to control the sample until it reaches the hood. The measures of transport and capture are capture velocity and face velocity, defined as follows.

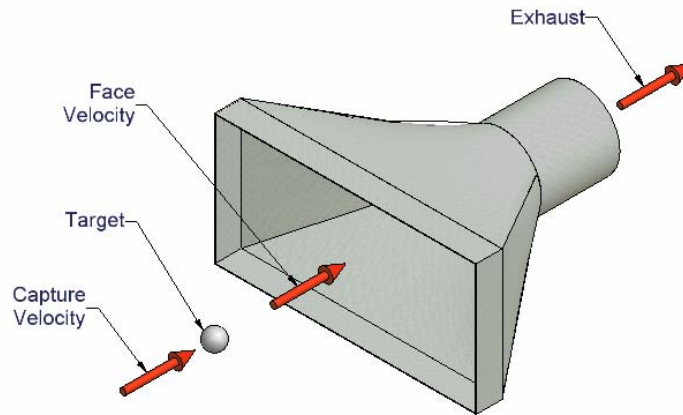
**Capture Velocity** – Minimum air velocity required to capture and transport a sample into the hood.

**Face Velocity** – Air velocity at the hood opening.



**Figure 3. Closed and Open Hoods**

Figure 4 shows the location of the capture and face velocities for an open hood.



**Figure 4. Capture and Face Velocities**

The volumetric flow rate,  $Q$ , for the local exhaust system is then defined as follows.

$$Q = V_f A \quad [3]$$

where,

$V_f$  = average velocity of hood face

$A$  = cross-sectional area of hood

Capture velocity is important when applying local exhaust ventilation to trace detection. Capture velocities typically range from 50 to 2000 feet per minute (fpm). The variability in capture velocity depends on several factors including: hood design (closed or open), type of sample to be collected (vapor or particulate), size and mass of sample, background air motion, and engineering judgment.

In addition to determining the capture velocity, understanding the principles of air movement are important. Figure 5 shows a fan with equal face velocities at the entrance (exhausting) and exit (blowing). In the blowing air stream at a distance of 30 outlet diameters, the velocity is approximately 10 percent of the face velocity and the airflow is directional. For the inlet flow, however, the distance is only one inlet diameter at 10 percent face velocity and the airflow is unidirectional. This shows the difficulty in influencing air movement by exhausting.

Capture velocity for an open hood with a rectangular inlet can be estimated using Equations 4 or 5.<sup>4</sup>

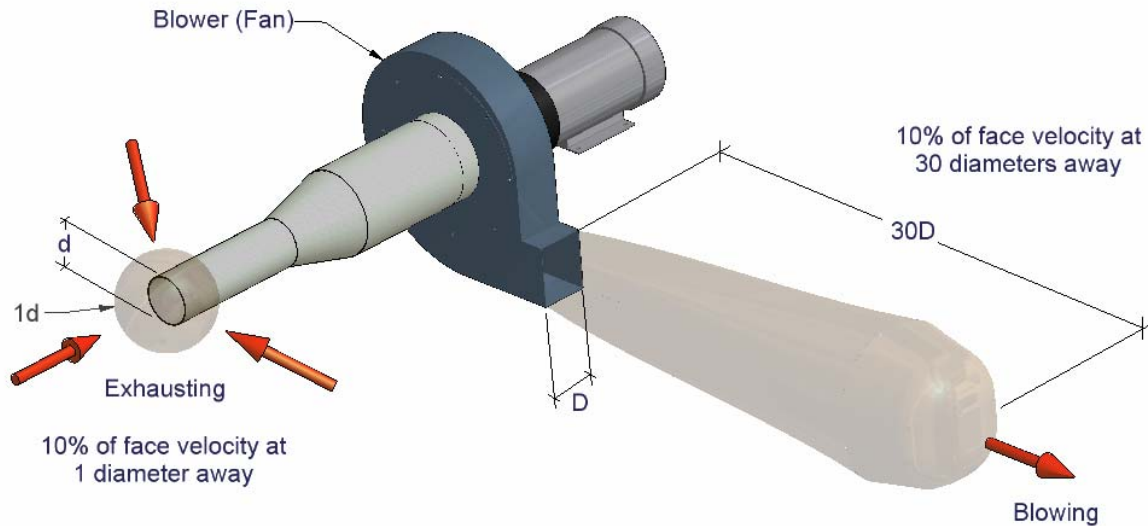
$$\text{Rectangular hood exhaust,} \quad V_c = Q / (10 X^2 + A) \quad [4]$$

$$\text{with baffles or flanges,} \quad V_c = Q / .75 (10 X^2 + A) \quad [5]$$

where,

$V_c$  = capture velocity at distance  $X$

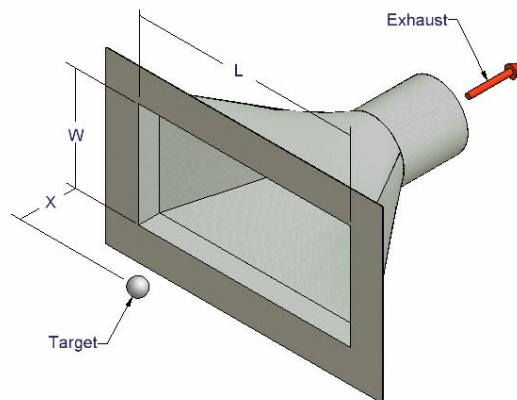
$X$  = distance from hood face to target



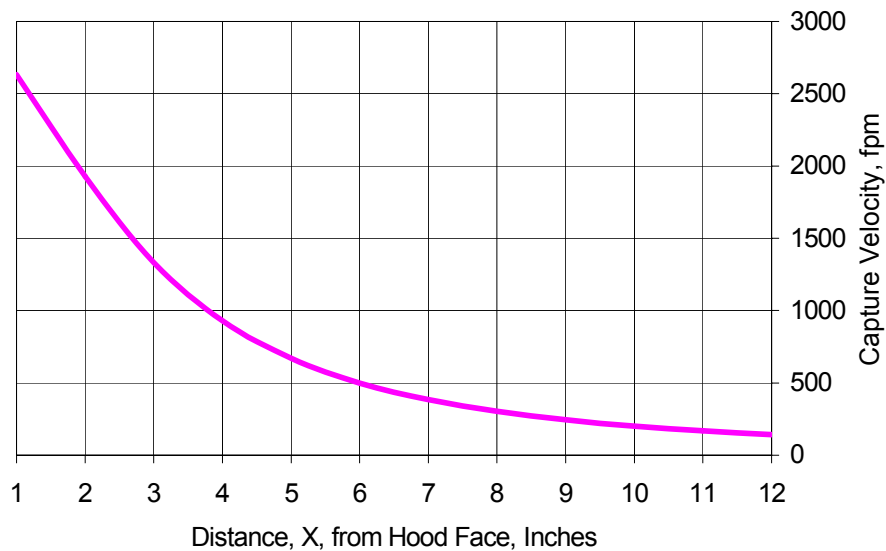
**Figure 5. Exhausting versus Blowing**

Rearranging Equations 4 and 5 to solve for  $Q$  shows that to maintain the same capture velocity at twice the distance (for example),  $Q$  quadruples. This further indicates the importance of locating the target and hood as close as possible. A better approach is to enclose the target, if appropriate, with a closed hood to improve sample collection. If enclosing the target is not possible, adding baffles or flanges parallel to the hood face can increase the capture velocity by approximately 25 percent by reducing airflow from behind the hood.

Applying Equation 5 to an example illustrates the effect on capture velocity and distance from the hood face. Figure 6 shows the example hood with a face opening of 6 inches by 12 inches and a face velocity of 3000 fpm. Figure 7 shows the resulting capture velocities as a function of distance,  $X$ .



**Figure 6. Open Hood with Baffles**



**Figure 7. Capture Velocity versus Distance from Hood Face**

In Figure 7, at 8 inches from the hood face, the capture velocity is 300 fpm or 10 percent of the face velocity. At this capture velocity, a sample released into a high airflow (e.g., spray painting) could be collected. At a distance of 12 inches, the capture velocity is 140 fpm and only a sample released into a low airflow (e.g. welding, plating) could be collected. To obtain these capture velocities, however, a fan system that will exhaust 1500 cubic feet per minute (cfm) would be required. At this exhaust flow and a moderate system pressure drop (7 inches of static pressure) through the hood, duct system, and filter, a 5-horsepower fan would be required. This example demonstrates the importance of localizing or enclosing the target to enhance sample collection and minimize fan power requirements.

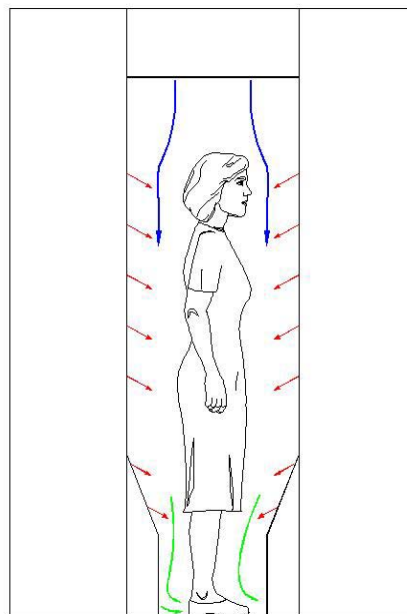
In a local exhaust ventilation system, the contaminant typically does not have a high velocity during its production; therefore, the airflow generated by the exhaust system can entrain and transport the contaminant easily. This is where the local exhaust ventilation system and trace detection system differ in their sample collection requirements. To dislodge an explosives sample (particulate) from a target requires external agitation. Because agitation applies momentum to the explosives sample, design considerations must be made in the sample collection system for trace detection. The factors include type of sample (small or large particles), velocity of the sample, background airflow, and hood design.

Sandia's explosives detection portal uses a patented sample collection method based on a modified open hood design called push-pull.<sup>6,7</sup> The portal sample collection system takes advantage of the airflow characteristics of exhausting and blowing shown in Figure 5. Figure 8 shows the airflow within the portal. Air curtain fans in the ceiling blow (push) directional airflow (blue arrows) over the body. Puffers in the wall (red arrows) provide external agitation to remove explosives sample. The removed explosives sample is entrained in the blowing airflow and carried to the floor where the unidirectional exhaust (green arrows) collects (pulls) the sample. With this collection method, washout through the portal's entrance and exit planes has been minimized. In addition, this method of sample collection has proved to be successful for collecting both explosives vapor and particulate with minimal fan horsepower.

The airflows within the portal have been designed to cover the complete body from head to feet. Sandia has demonstrated that the sample collection efficiencies between the head, body, and feet with this design are nearly identical. Therefore, if explosives are located at the head, body, and/or feet the portal can remove and collect samples. Because explosives may be located anywhere on a person, complete sampling of the body is required to enhance the probability of explosives detection.

For industrial application the typical volumetric air flows for local exhaust ventilation systems can range from hundreds to thousands of cfm. In the trace detection systems for which Sandia has applied the local exhaust method, large-volume sample collection has spanned from tens to hundreds of cfm. Compared to industrial applications, the Sandia systems have volumetric airflows several orders of magnitude lower. However, relative to typical sampling techniques for trace detection systems, these airflows are orders of magnitude larger.

Sandia has learned from developing the explosives detection portal that in addition to large-volume sampling to capture and transport a sample, large total volumes of air are required to obtain a minute explosives sample. The low concentrations of trace explosives, however, in the large-volume sampling airflow make direct detection difficult. Sandia has incorporated preconcentration in the large-volume sampling stream to increase concentration levels and make detection of very dilute explosives sample possible.

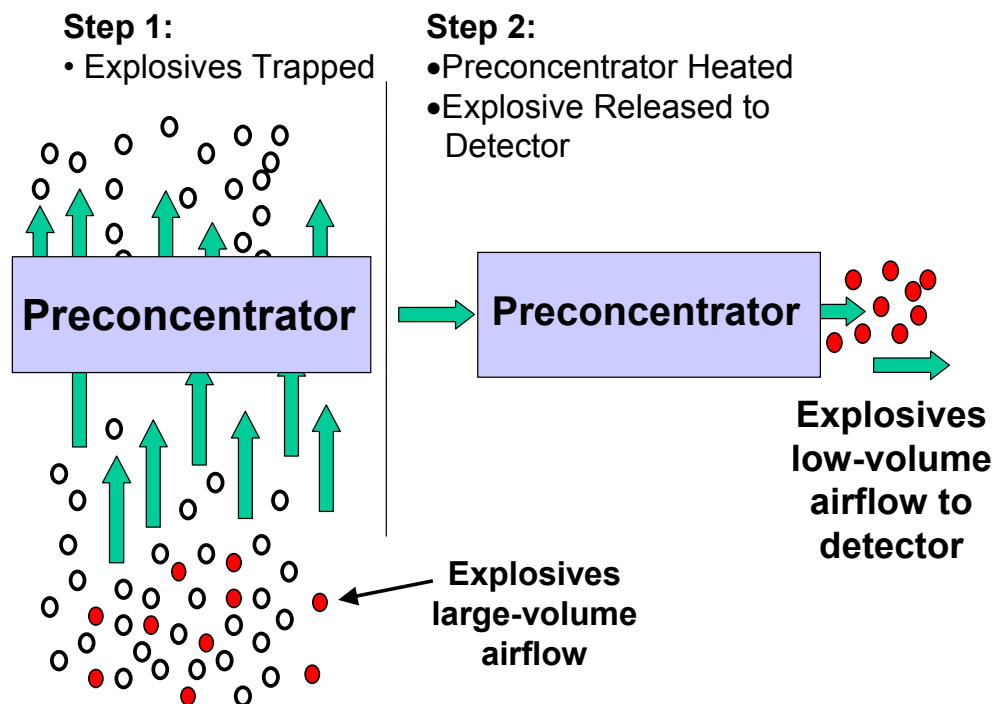


**Figure 8. Push-Pull Airflows in Sandia Portal**

## 4. Preconcentration

Sandia's large-volume preconcentrator is a mechanical system used to concentrate limited explosives samples. From a large-volume airflow, the preconcentrator adsorbs explosives sample (vapor or particulate) at room temperature. The adsorbing surface is then heated to desorb the explosives sample into low-volume airflow stream for delivery either to a detector or another preconcentration stage. Concentration of the explosives sample occurs because the explosives sample contained in the large volume prior to adsorption is now contained in a smaller volume after desorption. Equation 2 shows the relationship between concentration and volumes.

Figure 9 shows the operation of a large-volume preconcentrator. In Step 1, the preconcentrator intakes the large-volume airflow from the sample collection subsystem. Entrained in this airflow are minute amounts of explosives. In Step 2, the preconcentrator adsorption surface is heated to vaporize the collected and concentrated explosives sample into a low-volume airflow to the detector.



**Figure 9. Large-Volume Preconcentrator Operation**

The preconcentrator is a critical subsystem in a trace detection system because of its ability to collect small amounts of explosives from a large airflow. Without preconcentration the amount of material available to detect would be well below the limits of detection for many detectors. In addition, the preconcentration serves as an impedance-matching device between the large-volume airflow of the sampling system and the low-volume airflow to the detector. The requirements of a large-volume preconcentrator include:

- Inlet airflow to preconcentrator matched to outlet airflow of large-volume sampling
- Minimal pressure drop during large-volume adsorption, which reduces fan horsepower



- Minimal pressure drop during low-volume desorption, which reduces restriction to the detector inlet
- Minimal internal volume, which maximizes concentration,  $C$ , in Equation 2
- Efficient at absorbing and desorbing explosives, which maximizes,  $\eta_p$ , in Equation 2
- Desorb rapidly, which maximizes output concentration pulse
- Cycle quickly between adsorption and desorption, which maximizes system throughput
- Cost effective, easily maintained, and robust

Sandia has designed, fabricated, tested, and patented preconcentrators that meet these requirements.<sup>8,9,10</sup> These preconcentrators have been or are being used in several trace detection systems. Figure 10 shows the inlet size range of preconcentrators that have been developed. Table 1 indicates the large-volume airflows through the preconcentrators and approximate concentration factor.



**Figure 10. Sandia Large-Volume Preconcentrators (Inlet sizes: 9-inch, 6-inch, 2-inch)**

Table 1 shows that the large-volume airflows are approximately the same as the airflows previously described in sample collection. Matching output and input airflow optimizes the subsystem integration. By combining large-volume sampling and preconcentration, the ability to detect trace explosives has been significantly enhanced.

**Table 1. Characteristics of Sandia Preconcentrators**

Inlet Sizes inches	Large-Volume Airflow cfm	Concentration
2	120	~1,400
6	320	~3,800
9	680	~140,000*

\* Concentration ratio based on 2nd stage preconcentrator

## **5. Conclusion**

The importance of sampling and preconcentration at a systems level was presented using a mathematical model. Background for local exhaust ventilation systems was provided, as well as its application in trace explosives detection systems. It was shown that large-volume sampling is necessary in the collection and transport of sample. Finally, when large-volume sampling and preconcentration are integrated, the trace detection of explosives is greatly enhanced.

## 6. References

1. J. Yinon, *Forensic and Environmental Detection of Explosives*, John Wiley & Sons, 1999.
2. Rhykerd, Jr., C.L., Internal Report, *Performance and Recommendations for a Prototype for Automated Entry Control / Explosives Screening at High Security Checkpoints*, January 2001.
3. Rhykerd, Jr., C.L., Internal report, *Evaluation of Prototype Explosives Preconcentrators* (OUO), February 1996.
4. *Industrial Ventilation, A Manual of Recommended Practice*, 22nd Edition, American Conference Of Governmental Industrial Hygienists, 1995.
5. *Air Pollution Engineering Manual* (Second Edition), Los Angeles County Air Pollution Control District, Prepared For Environmental Protection Agency, May 1973.
6. Linker et al., *Vertical Flow Chemical Detection Portal*, United States Patent, No. 5,915,268.
7. Linker et al., *Target Detection Portal*, United States Patent, No. 6,334,365.
8. Linker et al., *Particle Preconcentrator*, United States Patent, No. 5,854,431.
9. Linker et al., *Particle Preconcentrator*, United States Patent, No. 6,085,601.
10. Linker et al., *Two-Stage Preconcentrator for Vapor Particle Detection*, United States Patent, No. 6,335,545.

**DISTRIBUTION:**

10	MS 0782	Kevin Linker, 4148
1	MS 0782	Rebecca Horton, 4148
1	MS 0768	Allen Camp, 4140
1	MS 9018	Central Technical Files, 8945-1
2	MS 0899	Technical Library, 9616
2	MS 0612	Review and Approval Desk, 9612, For DOE/OSTI