

HO-18-C043

# Analysis of Spread Index: A Measure of Laboratory Ventilation Effectiveness

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## ABSTRACT

*A laboratory ventilation system should limit the spread of contaminants and quickly purge the chemicals from a lab space to bring the concentrations at or below certain acceptable level. This study with the help of transient isothermal Computational Fluid Dynamics (CFD) analysis evaluates effectiveness of a laboratory ventilation system using two measures, namely, Spread Index  $(SI)_{TC}$  and Purge Time  $(PT)_{TC}$ .  $(SI)_{TC}$  quantifies how much of the lab volume is covered by an unacceptable level of concentration which is presumably the high risk concentration threshold (TC). Whereas  $(PT)_{TC}$  evaluates how much time it would take to purge the contaminants from the lab space to bring those concentration levels at or below the acceptable limit. The practical use of these indices are demonstrated by comparing the performance of two ventilation systems with two and three exhaust grills configurations. These analyses show  $(SI)_{TC}$  increases with the release of chemicals and reaches its peak until the release is stopped whereas  $(PT)_{TC}$  depends on the nature of the spread of contaminants. This analysis showed the distributed exhaust strategy with three exhaust grills significantly reduced the  $(SI)_{TC}$  values resulting in reduced concentration levels and chemical exposure (dose) of occupants. This study further indicates in spite of the well mixed airflow patterns the contaminant distribution especially in the breathing zone of the occupants is highly non-uniform. Interestingly the occupant closer to the exhaust grills shows high level of exposure than the one closer to the contaminant source. Therefore, control of lab environment by monitoring the concentration levels in the exhaust duct can compromise the safety of some occupants by under predicting their chemical exposure (does).*

## INTRODUCTION

The primary objective of laboratory ventilation systems is to provide a safe and comfortable environment to personnel. Simplistic approaches are often employed for specifying the supply air flow rate or air change rate per hour (ACH) for laboratory spaces in order to reach a certain level of dilution and target concentration of the contaminants. These approaches assume idealistic conditions of perfect mixing of contaminants with the supply air which presumably can yield uniform concentrations at or below the target concentrations in the entire space. Such well mixed conditions are rarely achievable even with the most simple lab layouts. In order to compensate for a variety of uncertainties, including imperfect mixing, safety factors are employed in the estimation of supply airflow rates which often result in specifying higher ACH (Feigley et. al. 2002). Once facilities are designed for high ACH they often continue to operate under the initial design conditions with the hope of achieving low uniform concentrations. Although high supply airflow rates can reduce the overall concentration of contaminants it may not ensure uniformity of concentrations at a low diluted level in the entire space. Importantly, locations of high contaminant concentration, especially those in the breathing zone (BZ) of occupants, can pose potentially higher risk of chemical exposure than other locations with average concentration. Under critical situations, such as in the case of accidental spill, it is important to control the strength and spread of such high concentration zones in a space and purge the chemicals quickly to bring the lab

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environment at the acceptable levels of concentration.

Air is the primary carrier of heat, moisture, and volatile contaminants in laboratory spaces. The distribution of supply air determines the resulting air velocities and the flow path of contaminants, which in turn, determines the distribution of temperature and concentration levels of contaminants in the space. Therefore, understanding the nature of airflow patterns and the flow path of contaminants can play a critical role in estimating the chemical exposure levels of workers at various locations in a laboratory. The dispersion of contaminants and their flow path can depend on several inter-related factors including the location and type of supply diffusers, supply air flow rates and associated diffuser throws, supply air temperature, size and locations of room return, locations and strengths of various heat sources in a room, floor layout including the location and size of fume hoods, location of work benches and any other obstructions to airflow, and importantly on the strength, location, and source of contaminants.

Jin et. al. (2012) performed experimental investigation of a mockup laboratory setup to evaluate the impact of exhaust locations and the chemical spill positions on the distribution of contaminant concentration. They concluded that ACH can be reduced without increasing the safety risk if the ventilation system is properly designed. Their results showed if the chemical source is moved closer to the exhaust or if local bench hood exhaust is utilized the concentrations can be effectively reduced without increasing the ACH. A steady state isothermal Computational Fluid Dynamics (CFD) study performed by Feigley et. al. (2002) showed excellent agreement between the predicted and experimentally measured concentration of contaminants. Their study involving wide combination of airflow rates, exhaust and spill locations predicted high level of non-uniformity in the contaminant concentrations. They too concluded that concentration levels in the room dependent on the airflow patterns which varied with the location of supply diffuser, exhaust grill, and source. Klein et. al. (2009) performed chemical spill tests through a controlled release of organic solvents in a laboratory space and measured transient variations of chemical concentration under various supply airflow rates. They concluded the maximum improvement in lowering the concentrations occurred between 6 and 8 ACH with diminishing returns for ACH greater than 12. They noted that location, number, and style of supply and return diffusers can effectively increase the laboratory ventilation efficiency and can potentially allow for lower ACH. Previous CFD analysis implied that the flow path of contaminants has larger impact on the distribution of contaminant concentrations and laboratory ventilation effectiveness than supply airflow rates (Khankari, 2016).

This paper with the help of CFD simulations investigates the transient dispersion of contaminants in a laboratory space under a control release of contaminant. Two measures, namely, Spread Index  $(SI)_{TC}$  and Purge Time  $(PT)_{TC}$  are introduced to evaluate the effectiveness of laboratory ventilation systems. Spread Index  $(SI)_{TC}$  quantifies the extent of a laboratory volume covered by an unacceptable level of concentration which is presumably the high risk concentration threshold (TC) whereas Purge Time  $(PT)_{TC}$  analyzes the time it would take to bring the concentration levels at the desired level after release of the contaminants. These indices are used to test the ventilation effectiveness of two HVAC configurations.

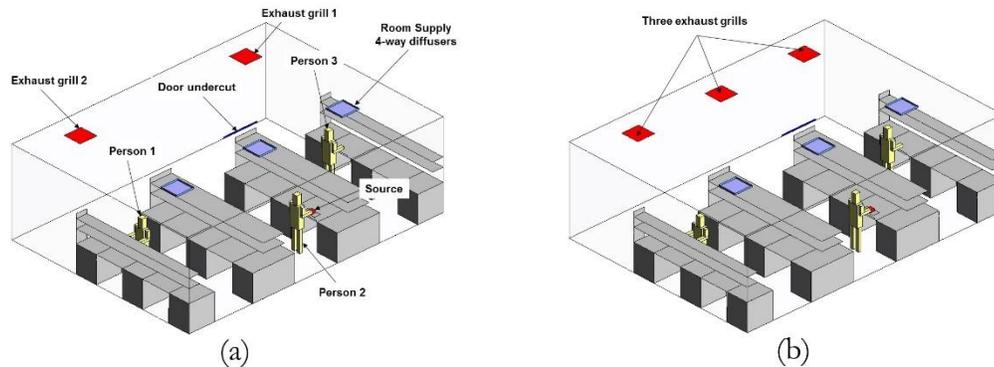
## **VIRTUAL LABORATORY SET-UP**

A three-dimensional, transient, isothermal Computational Fluid Dynamics (CFD) model of a laboratory is developed for this study. The laboratory has about 660 sq. ft. ( $61.3 \text{ m}^2$ ) floor area (30 x 22 feet, 9 x 6 m) with 9.5 feet (2.9 m) ceiling height. As shown in Figure 1 the virtual laboratory has three rows of work benches and three occupants located at various locations. Figure 1b shows another case where an additional exhaust grill is placed in the middle row. This HVAC configuration is referred as “distributed exhaust” case.

The outside air is supplied at an angle of 15 degrees through a set of three 4-way overhead diffusers located over the work benches. Traditionally such type of diffusers are employed to enhance the mixing. The room air is exhausted through the exhaust grills placed in the ceiling. The chemical spill is simulated as a source of a hypothetical chemical vapor with a constant release rate of 7 mL/s ( $7.0\text{E-}06 \text{ m}^3/\text{s}$ ) for the duration of 12 minutes. As shown in Figure 1a the source of contaminant is placed on the bench in the vicinity of the person 2.

The transient analysis was performed for a total duration of 60 minutes with the supply airflow rate of 6 ACH (590

cfm, 278.5 l/s). The room is operated at slightly negative pressure and the makeup air is supplied through the gap under the room door. The makeup air flowrate was maintained at 100 cfm (47.2 l/s). Virtual sensors were placed in the model in front of each occupant's face as well as in the two exhaust grills to monitor time varying chemical concentrations at each location. With the help of this data the chemical exposure (dose) for each occupant was computed by the cumulative product of the chemical concentration (ppm) and the duration of the exposure (min). The standard k-ε turbulence model was employed to compute the turbulent viscosity of the air. A computational mesh of 1.2 million hexahedral mesh was created by placing fine mesh near the strategic locations. Numerical computations were performed using ANSYS Fluent commercial CFD software.



**Figure 1:** Schematic diagram of CFD models of a laboratory: a) base case HVAC configuration with two exhaust grills b) distributed exhaust case with three exhaust grills.

**Spread Index  $(SI)_{TC}$ :** is the ratio of the volume of the room occupied by contaminants above a certain target concentration (TC) to the total volume of the room. Ideally the lab ventilation systems should minimize the chemical concentrations levels below the desired target concentration everywhere in the lab space and should limit the spread of contaminants above the desirable level. Thus, Spread Index  $(SI)_{TC}$  helps in analyzing and quantifying the extent of spread of contaminants in the room above the desirable target concentration. Assuming the target concentration is a safe exposure limit then ideally the contaminant concentration should remain below the target concentration everywhere in the lab space. It means ideally the  $(SI)_{TC}$  should be close to zero every time during the lab operation. It should be noted that the safe level of concentrations can depend on several risk factors including the type and quantities of chemicals utilized in the labs and their safe exposure limits. Therefore, for each laboratory  $(SI)_{TC}$  can be evaluated for various levels of target concentrations based on the chemical exposure risk analysis. High values of  $(SI)_{TC}$  can indicate spread and build-up of contaminants above the safe levels of the concentration. The design of a HVAC system and the resulting flow path of contaminants would play an important role in determining the  $(SI)_{TC}$  levels in the space (Khankari, 2016). For this study the target concentration is assumed to be at 25 ppm, and hence,  $(SI)_{25}$  is analyzed.

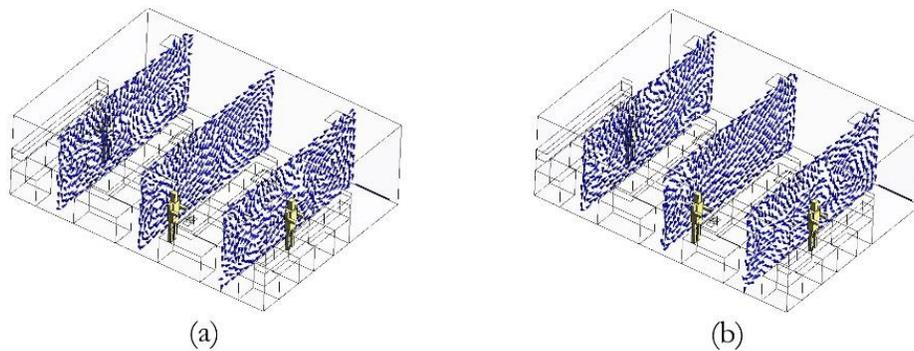
Since the chemical concentration level in the breathing zone is the most important parameter which directly affects the occupants exposure, it is possible to compute a subset of  $(SI)_{TC}$  limited only to the breathing zone instead of the entire lab volume. It should be noted that it is possible only with the help CFD simulations to estimate  $(SI)_{TC}$  and visualize such a volume of high concentration which otherwise is almost impossible to measure and visualize in the real world.

**Purge Time  $(PT)_{TC}$ :** is the time that a ventilation system requires to reduce the Spread Index  $(SI)_{TC}$  from its maximum value to zero. In other words  $(PT)_{TC}$  is a measure of the effectiveness of ventilation system in clearing the lab space of hazardous contaminants and bringing the concentration to an acceptable level (target concentration).  $(PT)_{TC}$  can provide valuable guidance in determining the safe period during which occupants can be evacuated after an

accidental spill of chemicals. Also in the case of demand control ventilation HVAC systems  $(PT)_{TC}$  can help in determining the supply airflow rates during the ramp up phase.

## RESULTS AND DISCUSSION

Figure 2 shows the airflow patterns at three vertical planes in the lab. As shown in these figures the air exiting from the diffusers travels along the ceiling, descends along the walls and moves inward away from the walls. Such airflow patterns create large recirculation loops in the vicinity of the walls. Part of this recirculating air escapes through the exhaust grills. As shown in Figure 2b addition of an exhaust grill provides an easy escape path for the air in the central section of the lab. Three dimensional airflow patterns (not shown here) are quite complex which promote mixing in the entire lab space as expected from the 4-way ceiling diffusers.



**Figure 2:** Airflow patterns at three different vertical planes at 5.3 ft (1.6m), 15 ft (4.5 m), 24.75 ft (7.5m) in a lab: a) base case b) distributed exhaust.

Figure 3 shows the concentration of contaminants at a breathing zone height of 5 foot (1.5 m) after 720 s of release of contaminants. Figure 4 shows associated cloud of 25 ppm (and higher) concentration in a three dimensional space of the lab. Such cloud depicts the three dimensional spread of the contaminants in a lab above the acceptable level of 25 ppm. These figures show non-uniform distribution of contaminants in the lab space which contradicts the traditional belief of “well mixed” uniform conditions. In spite of the mixing airflow patterns the contaminant distribution is not uniform. In a real life such “well mixed” conditions can probably occur only in the exhaust ducts.

As shown in Figures 3 and 4 the zone of high concentration (25 ppm and higher) tends to drift towards the exhaust grill located near the door undercut. This grill is also closer to the source of contaminant than the other grill in the opposite corner. As a result the concentration levels in the first row of the benches are lowest compared to those in the second and third row. It should be noted in the case of two exhaust grill scenario the face of the third occupant located in the third row is immersed in the zone of high concentration. As shown in Figure 3b and 4b an addition of the third exhaust grill reduces the concentration levels both in the first and the third row. As a result the concentration levels in the vicinity of the second person (closer to the contaminant source) are increased. It should be noted that the spread of contaminants above the undesirable concentration levels reduced by addition of the third exhaust grills. By addition of the third grill the  $(SI)_{25}$  after 720 s of release of contaminants reduces from 16 to 11 percent.

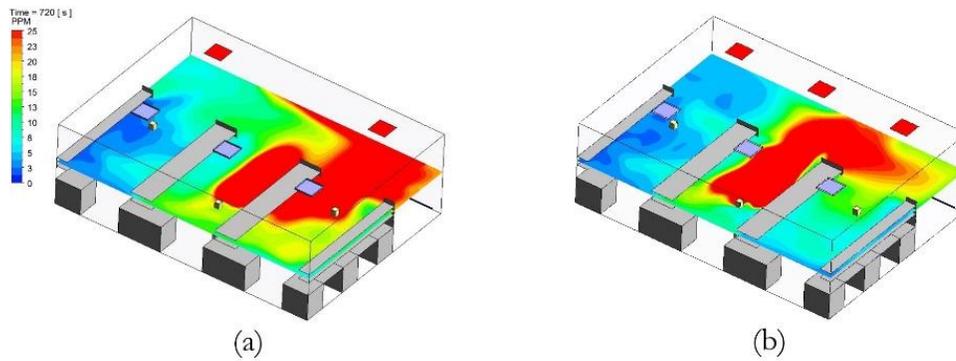


Figure 3: Distribution of contaminant concentration at the breathing zone after 720 s of release of contaminant, a) base case b) distributed exhaust

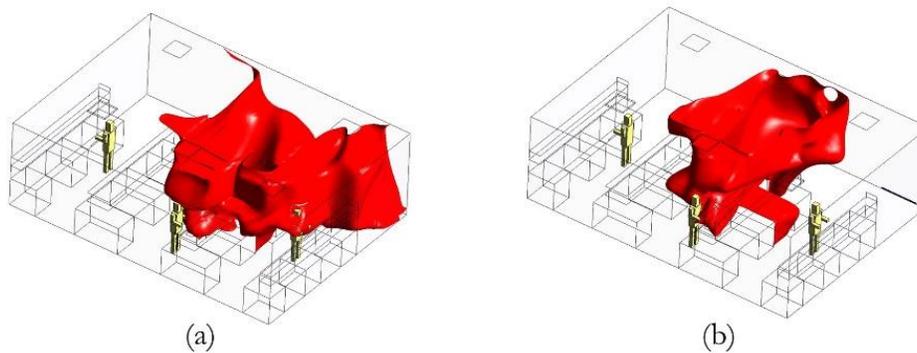


Figure 4: Cloud of 25 ppm concentration showing the spread after 720s release of contaminant, a) base case b) distributed exhaust.

### Analysis of Spread Index (SI)<sub>25</sub> and Purge Time (PT)<sub>25</sub>

Figure 5 shows variation of Spread Index (SI)<sub>25</sub> with time for two and three exhaust grills (distributed exhaust). As shown in this figure the (SI)<sub>25</sub> values (spread of contaminants) increase with the release of contaminants and reach the peak at 12 minutes when the release of the chemical vapors stops. After this time the (SI)<sub>25</sub> values show sharp decline and reach zero level at about 25 minutes. It means at this time the concentration levels everywhere in the lab space are below the hazardous threshold of 25 ppm. The volume the lab space occupied by the undesirable contaminant concentration level (25 ppm) gradually increases until the release of the contaminants stops and then it starts decreasing until the chemicals are purged from the space. It is interesting to note that the peak value of (SI)<sub>25</sub> reduces from 26.6 to 16.4 percent by just adding an extra exhaust grill. It indicates the strategy of distributed exhaust can help in controlling the spread of contaminants above the undesirable levels.

In the case of two exhaust grills scenario it takes about 420 s (Purge Time) for the ventilation system to bring the contaminant concentration from its peak value to the desirable level of less than 25 ppm. Whereas in the case of distributed exhaust (three grills) it takes 720 s (300 s more) for the same to occur. The in-depth analysis of the variation

of 25 ppm cloud indicated that in the case of distributed exhaust the chemical vapors were trapped under the benches which took longer to purge (Figure 4b). Otherwise this analysis indicates that in the case of distributed exhaust design the  $(SI)_{25}$  value reaches to about 0.01 from 0.16 in 420 s which is almost similar to the two exhaust grill. It indicates that the nature of distribution of contaminants can affect the Purge Time  $(PT)_{TC}$ . It would take longer to clear the trapped contaminants under the benches or within other structural components.

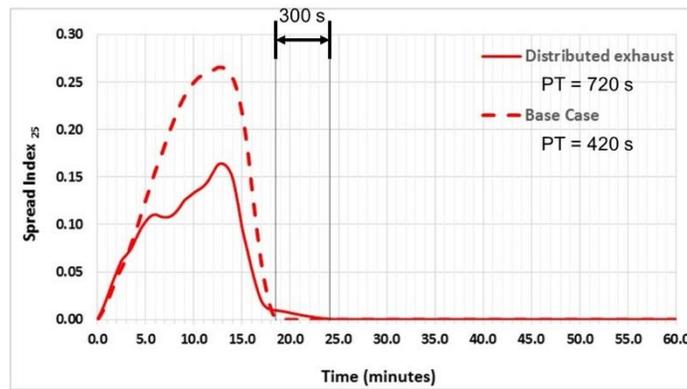


Figure 5: Variation of Spread Index  $(SI)_{25}$  with time for the base and distributed exhaust configuration.

### Analysis of Chemical Exposure (Dose)

Figure 6 shows variations of chemical concentration with time in front of each person’s faces as measured by virtual sensors. This figure also compares the similar transient variation of concentrations in the exhaust duct computed from the sensors located in the exhaust grills. It shows the concentration levels in the exhaust duct can significantly vary from those in the breathing zones of occupants. The concentration level in front of each person starts increasing with the release of the chemicals, reach certain peak value, and then starts decreasing. The peak values of the concentration and the time at which those occur vary depending on the location of the occupant. In the case of person 1 and person 3 who are away from the source the peak values are lower than the person 2 who is closer to the source. Similarly the peaks in the concentration levels for the person 2 occur sooner than those for the other two occupants. It shows the concentration levels in general reduce by addition of an extra exhaust grill. In the case of person 2, however, the concentration levels for the case of three exhaust grills are higher during the initial release phase. This might be due to local buildup of chemical vapors during the initial release of chemicals. It is also interesting to note that the impact of number of grills on the concentration levels is more significant during the initial ramp up phase than during the ramp down phase.

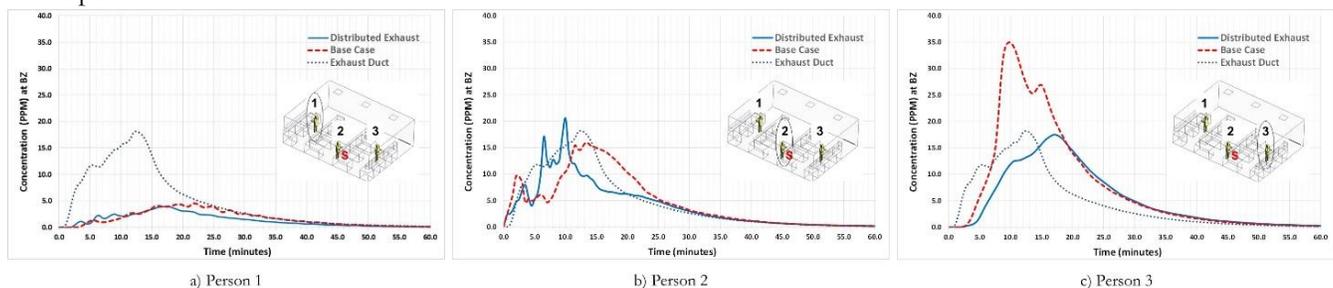
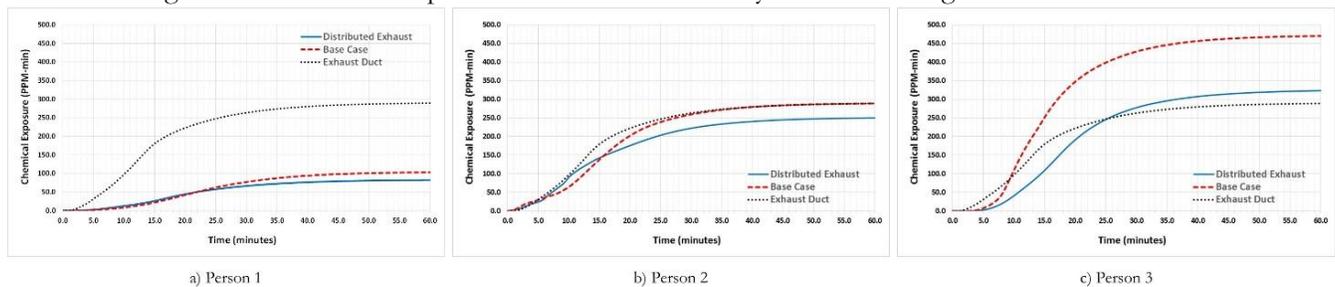


Figure 6: Variation of contaminant concentrations with time in front of the faces of occupants and in the exhaust duct.

Figure 7 shows variations of the cumulative chemical exposure (dose) with time for each occupant computed from the concentration levels shown in Figure 6. These figures also compare the dose levels computed from the concentrations in the exhaust duct. It shows occupant exposure estimated from the exhaust duct concentration can be misleading – a few occupants would be under exposed while a few would be over exposed. Therefore, the design and control of HVAC systems based on exhaust duct concentrations cannot ensure the safe environment for all occupants.

Figure 7 shows the cumulative chemical dose (ppm-min) for each occupant increases rapidly during the initial release phase; and then reaches certain peak value; and remains almost constant thereafter as the chemical concentrations start decreasing. It is counter intuitive to note that the Person 3 near the exhaust grill in the third row shows higher level of exposure than the one closer to the source. However, addition of an exhaust grill (distributed exhaust) reduces the exposure levels for all the occupants which corresponds to lower values of  $(SI)_{25}$  for the distributed exhaust. Such reduction is significant in the case of person 3 who is in the vicinity of the exhaust grill.



**Figure 7:** Variation of chemical exposure (dose) with time for each person.

## SUMMARY AND CONCLUSIONS

A virtual laboratory setup is developed with the help of Computational Fluid Dynamics (CFD) models to analyze the transient dispersion of contaminants in a laboratory space under a control release of contaminant. The ventilation effectiveness of the HVAC system is analyzed with the help of two measures, namely, Spread Index  $(SI)_{TC}$  and Purge Time  $(PT)_{TC}$ .  $(SI)_{TC}$  quantifies the extent of the room volume covered by unacceptable concentration level which is presumably the high risk concentration threshold. Whereas  $(PT)_{TC}$  evaluates the time required to purge the contaminants from its highest  $(SI)_{TC}$  value to zero. Additionally the performance of the ventilation system with two and three exhaust grills (distributed exhaust) is compared using these indices.

These analyses indicate the transient distribution of contaminants can be highly non-uniform in spite of the “well mixed” airflow patterns. Such non-uniformity especially in the breathing zone can expose the occupants to various degrees of health risks. This analysis showed occupants closer to the exhaust grill can be exposed to a higher level of risk than the one closer to the source of contaminant. It further indicated that monitoring of lab environment using concentration levels in the exhaust duct can compromise the safety of occupants. Due to highly non uniform nature of the contaminant distribution it can under predict the chemical exposure (does) for some occupants.

The analysis of Spread Index  $(SI)_{TC}$  showed the volume of the room occupied the chemicals above certain threshold concentration level increases with the release of the chemicals, reaches its peak until the release is stopped, and then, shows sharp decline. The Purge Time  $(PT)_{TC}$  – the time required to bring the concentration levels below certain acceptable threshold depends on the nature of the contaminant distribution. It would take longer to clear the trapped volumes in the space. However, just addition of an extra exhaust grill significantly affected the contaminant distribution in the space resulting in reduced concentration levels and chemical exposure (dose) of occupants. It seems distributed exhaust strategy can help in reducing the chemical exposure risks in laboratories.

It should be noted that several factors can determine the effectiveness of the lab ventilation systems. Therefore, it

is difficult to reach to any general conclusions about the optimized design and operating conditions. However, as demonstrated in this CFD study the  $(SI)_{TC}$  and  $(PT)_{TC}$  indices can be effective tools for a strategic design of a laboratory ventilation systems to minimize the chemical exposure risks of occupants.

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