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A Study of Refrigerant Dispersion In Occupied Spaces Under Parametric Variation

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Abstract

While an understanding of the dispersion of refrigerant in occupied spaces is important to ASHRAE Standard 15-2010's objective of ensuring the safety of occupants for spaces in which HVAC&R systems are installed, only simplified models are generally used to describe refrigerant leakage phenomena because of their complexity. This paper describes some studies of the transient refrigerant dispersion behavior from variations in the leakage rate, the exhaust ventilation rate, and the height of a wall undercut that could be used to develop improved models of the dynamics of refrigerant leaks. The results indicate that well-mixed models do not accurately describe the refrigerant distribution in many cases because of stratification, and that this stratification may be used in tandem with vent placement to ensure that refrigerant concentration levels do not exceed safety limits.

1 Introduction

One long-standing and significant concern for engineers designing, specifying, and installing refrigeration and air-conditioning systems is the effect of refrigerant leaks on the health and well-being of affected building occupants. ASHRAE Standard 15-2010 (2010), *Safety Standard for Refrigeration Systems*, was originally developed 100 years ago to address these concerns by specifying guidelines for the permitted installation of these systems that would minimize risk to room occupants by imposing limits on the amount of refrigerant permitted for these types of systems and specifying other aspects of system-level design. This standard has been regularly updated to account for advances in HVAC&R technology, and is now prescriptively applied to a wide range of systems to ensure occupant safety for spaces through which refrigerant pipes travel.

Because the physical phenomena that govern the transient refrigerant distribution in occupied spaces are quite complex, Standard 15 uses simple models of leakage phenomena to prescribe safety guidelines. As an example, this standard imposes stringent limits on the total mass of refrigerant (i.e., the refrigerant concentration limit (RCL) set by ASHRAE Standard 34-2010 (2010)) in the installed system that could potentially enter the space without considering the refrigerant leakage rate into the occupied space, which is affected by a wide range of factors. While such simple models are certainly quite useful in this application, they tend to produce extremely conservative safety criteria that may affect the installation of HVAC&R systems in particular applications. Questions can therefore arise when applying these guidelines to new innovative systems developed by the HVAC&R industry since the development of Standard 15, such as VRF systems (Duda, 2012), since there are significant differences between the architecture of these new systems and the architecture of the more conventional chilled-water systems for which Standard 15 was originally written. Research incorporating new information about equipment construction, installation, and operation that would result in more realistic refrigerant dispersion models, without compromising the practical nature of Standard 15, could have a significant impact upon HVAC&R systems in buildings (Waye et al., 2012).

One potential approach for achieving this goal involves partitioning it into two separate objectives: determining the appropriate leakage rate for a given system and failure mode, and determining the effect of the space's geometric parameters on the refrigerant dispersion for a given leak rate. Rather than assume that a system's charge instantaneously appears in the occupied space, research that analyzes the effects of both the architecture of the particular cycle in consideration, such as piping restrictions and expansion devices, and possible failure modes, such as the size of fatigue-induced cracks, can provide a scientific basis for these leakage rates that might be observed in the field. In addition, research into the sensitivity of the transient refrigerant dispersion to a common set of geometric parameters, such as the room size, ventilation rates, and the size of door undercuts and connecting spaces, will engender a new understanding of the features of spaces that determine their compatibility with different system types. By pursuing such a two-fold approach to understanding the dynamics of refrigerant dispersion in occupied spaces, it will be possible to create more realistic bounding scenarios that can be use in rigorous fault tree analyses for Standard 15, and engineers and system designers will be able to make both existing and new systems more energy efficient and effective at achieving occupant comfort, ensure the safety of building occupants, and facilitate the specification and inspection of these systems by local code enforcement authorities.

Recent interest in understanding the behavior of flammable refrigerant leaks has resulted in a number of publications that are relevant to this topic. Kataoka et al. (1999) studied different refrigerant releases in occupied spaces both in simulation and in experiment, and explored a variety of types of parametric variation, such as the refrigerant leakage rate and the leakage height. Other recent publications by Nagaosa et al. (2012), Lewandowski and Reid (2012), Hihara (2014), and Okamoto et al. (2014) also study the dynamics of refrigerant dispersion; however, the focus of their work is the possibility of combustion for a variety of working fluids, rather than studying the transient behavior of the refrigerant concentration in the space.

The objective of this paper is the study of refrigerant dispersion in a single occupied space to provide a greater understanding of the dependence of the transient refrigerant flows upon a set of geometric parameters, such as door undercut height or the exhaust ventilation flow rate. A particular emphasis is placed on exploring phenomena, such as the level of stratification, that will affect the validity of candidate models for describing the refrigerant distribution. Section 2 presents the assumptions used to construct the computational fluid dynamics (CFD) simulations. In Section 3, we discuss a series of simulations conducted on refrigerant leaks in a single space. We then present a brief overview of some mathematical techniques that can provide new analytical insights into the refrigerant mixing phenomena in Section 4, and finally discuss a set of conclusions and perspectives on future work in Section 5.

2 CFD Background

This initial study of refrigerant dispersion dynamics is focused on a single occupied cubic space that is 10 feet on a side, which is similar to many small hotel rooms. Such a space provides a useful limiting case in which to judge the dynamic behavior of the refrigerant concentration during a dispersion event. These simulations were configured with a refrigerant leak located in the middle of the ceiling, such as might occur in the placement of a VRF ceiling cassette unit, with a leakage mass flow rate of $\dot{m}_{leak}$

flowing through an axisymmetric source of diameter $D = 0.5$ inch. The total mass of refrigerant injected into the room during these experiments, 40 pounds, was also chosen because it is representative of a large VRF system. There are two means by which the refrigerant can exit the room: either through an exhaust fan, with a constant flow rate of Q_{exh}, located 12 inches from each side wall on the ceiling in the upper corner of the room, or through a wall undercut, which connects the occupied space with an adjacent empty space, spanning the length of the room and has a height of h_{out}. An undercut spanning the full width of the wall was used instead of a partial-width undercut, as would be located under a door, because the smoothness of the computational mesh. A series of computational studies were performed to assess the impact of this undercut width on the fluid dynamics which demonstrated that the difference in the simulations were negligible because the velocity fields are mainly sensitive to the height of the undercut, rather than its width. Using the terminology thus described, this paper will investigate the time-varying refrigerant concentration in the room as a function of $\dot{m}_{leak}$, Q_{exh}, and h_{out}.

Computational fluid dynamics (CFD) simulations were used to study the temporal and spatial development of the velocity, concentration, and temperature fields of an air/refrigerant mixture. An ideal gas model of air was used, while a real gas model of the refrigerant R410a was used to describe the leaking fluid. Under the further assumption that the air/refrigerant mixture is a Newtonian two-component fluid, the governing equations consist of the Navier-Stokes equations (continuity and conservation of momentum) along with the conservation of energy, conservation of species and the two-equation model (k–ω) as the turbulence closure in a three-dimensional space (Bird et al., 2006). The governing equations were iteratively solved by the commercial code ANSYS CFD (CFX 15.0), which implements the finite volume method on an unstructured 3-D mesh. A higher-order scheme was used to describe the convective and diffusive terms, and a second-order backward Euler method was implemented for temporal discretization (Ans, 2014).

One aspect of the CFD simulations that required particular attention was the construction of the computational mesh on which the equations were solved. Since the domain of the computations included regions of high velocity and turbulence, mesh refinement was applied to these crucial regions of the domain to capture the main features of the flow without incurring high computational costs. A grid-convergence study was also conducted, in which the grid size was varied from 2.51E+5 to 1.71E+6 elements, to determine the proper grid density. The temporal step-size was also evaluated to ensure that unphysical oscillations in the refrigerant concentration in the breathing zone due to numerical dispersion are significantly smaller than main features of the flow. As a result of this study, calculations were all performed with a grid system of the $N \sim \mathcal{O}(10^5)$ and $\Delta t \sim \mathcal{O}(10^{-1})$. An adaptive time-stepping method was applied to avoid numerical instabilities, which leads to significantly smaller values of Δt at the beginning of the simulation.

3 Refrigerant Dispersion in a Single Room

Because of the complex dependence of the transient refrigerant velocity and concentration fields on the variation in the geometric parameters, the results from varying each geometric parameter will be discussed in sequence. The effect of the refrigerant leak rate will be presented first, due to its dominant influence; two leak rates are examined, $\dot{m}_{high}$ (25% of system charge in 1 minute, or 75 g/s) corresponding to the leak rate proposed in Appendix E of UL 484, and $\dot{m}_{low}$ (10 kg/hr, or 2.5 g/s) corresponding to the leak rate proposed in ISO 5149. The effect of varying both h_{out} and the Q_{exh} on the transient

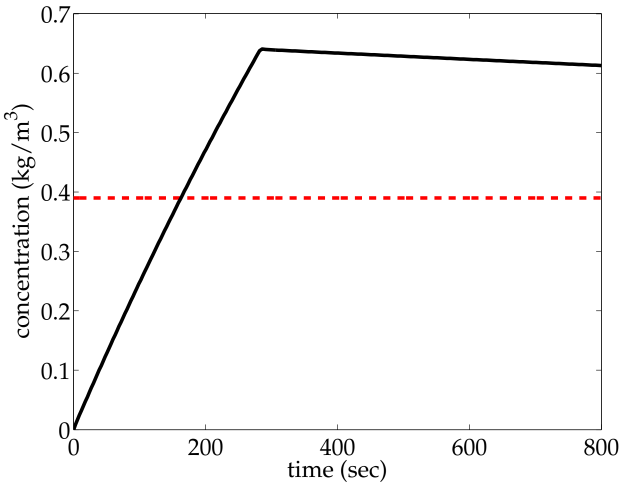

Figure 1: $\overline{C}$ during a high-rate leak, with a $Q_{exh} =$ 5cfm and h_{out} = 0.25in, over 800 seconds. The RCL is denoted by the dashed line.

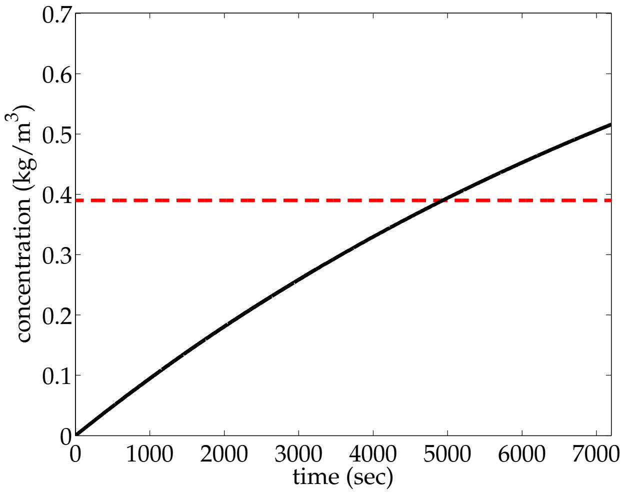

Figure 2: $\overline{C}$ during a low-rate leak, with $Q_{exh} =$ 5 cfm and h_{out} = 0.25 in, over 7200 seconds. The RCL is denoted by the dashed line.

refrigerant concentration in the occupied space will then be presented.

A variety of metrics and criteria were used to analyze the data generated in these simulations. The first and most important such metric was the RCL (390g/m^3 for R410a), which allows for the straightforward calculation of the maximum refrigerant mass that can be permitted to enter a space while maintaining a safe environment for room occupants. Because this metric does not incorporate the notion of "exposure time", this study also analyzed the time-varying spatially-averaged refrigerant concentration $\overline{C}$, computed by

$$\overline{C} = \frac{\iiint_V C(x,y,z)dV}{\iiint_V dV}, \tag{1}$$

for each case of the desired parametric variation. Since $\overline{C}$, like the RCL, does not provide information about the spatial variation in the refrigerant concentration throughout the space, the local refrigerant concentration is also studied in a few localized regions in the room, including the area in front of the exhaust vent and the area in front of the wall undercut. The local concentration over the exhaust area is defined by

$$C_{exh} = \begin{cases} \frac{\int\int_A \dot{m} C dA}{\dot{m}} & : v \cdot \hat{n} \geq 0 \\ 0 & : v \cdot \hat{n} < 0, \end{cases} \tag{2}$$

while a similar definition of C_{out} is defined for the undercut. These local concentrations can then be compared to the spatially averaged concentration $\overline{C}$.

Figures 1 and 2 illustrate the results of using CFD simulations for the $\dot{m}_{high}$ and $\dot{m}_{low}$ scenarios, in which Q_{exh} was held constant at 5 cfm and h_{out} = 0.25 inch. Focusing first on the $\dot{m}_{high}$ scenario illustrated in Figure 1, it is clear that the concentration quickly reaches the RCL, and that it increases in a nearly linear fashion until the 40 pound system charge is depleted. At the time of leak cessation t_f, the room contains a high concentration of refrigerant which results in the exchange of the air/refrigerant mixture with the exterior through the small gap at floor and also the exhaust vent at the ceiling.

One particularly notable feature of these dynamics is that the high-density refrigerant flow takes the form of a buoyant downward jet. As the jet descends toward the floor of the room, ambient air is

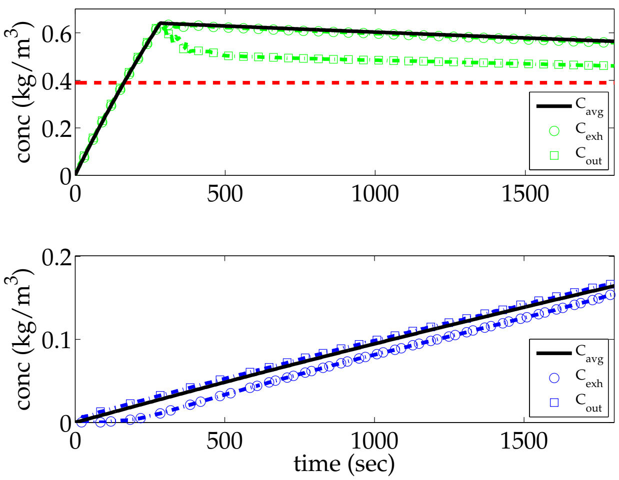

Figure 3: $\overline{C}$ compared to the local concentrations C_{exh} and C_{out} for the high-rate leak (upper plot) and low-rate leak (lower plot).

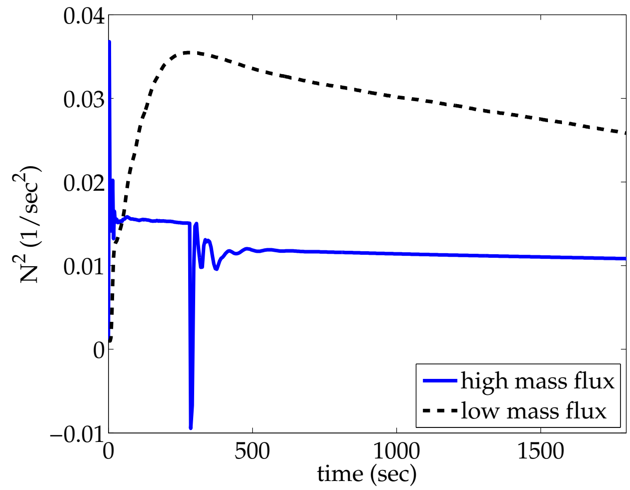

Figure 4: Buoyancy frequency indicates significant stratification.

entrained so that the concentration in the centerline of the jet decreases. This jet then spreads out toward the end walls when it reaches the floor of the room, increasing the density at the lower room elevations. This entrainment continues with the lateral discharge of the buoyant jet, so that a transient stratification of the refrigerant in the room develops in a manner similar to a filling-box process (Nabi and Flynn, 2013). Over time, the higher concentration accumulates at the bottom of the room and advects upward in the room while the jet descends, during which time the make-up air also enters the room in a form of ascending plume from the undercut.

The particular characteristics of this filling-box process can have a significant effect on the degree to which the concentration field is stratified. The amount of stratification can be qualitatively assessed by comparing the magnitude of the gravitational forces to the magnitude of the source momentum flux, which is itself proportional to $\dot{m}_{leak}$. Large values of this ratio indicate that the room is highly stratified, while small values indicate that the room is not stratified. Smaller values of $\dot{m}_{leak}$ will therefore result not only in lower average values of refrigerant concentration, but also in a higher level of stratification. This stratification can also result in different concentration profiles between locations high in the room (exhaust vent) and locations low in the room (undercut).

Due to the high computational cost that accompanies the use of CFD, one popular simplifying modeling assumption for these applications is that the room air is well-mixed, which causes the time-varying refrigerant concentration in the space to be spatially uniform. While the resulting models are much easier to formulate and simulate than CFD models, it is essential to understand the degree to which the refrigerant concentration is stratified so as to assess the potential validity of these models for this application. The spatially averaged concentration $\overline{C}$ in the $\dot{m}_{high}$ simulation is therefore compared to C_{exh} and C_{out} in Figure 3. It is clear from this figure that the concentrations C_{exh} and C_{out} are nearly identical to $\overline{C}$ for $t \leq t_f$, but that the local concentrations quickly diverge after the cessation of the leak. This qualitatively validates the proposed dependence of the mixing on the momentum flux as described above, and also highlights the importance of accounting for the effect of even 5 cfm of make-up air that enters due to Q_{exh} and the undercut. Moreover, this also provides qualitative guidance for refrigerant leak mitigation strategies; if one assumes that the leak rate is very high, then the success of these strategies is not dependent on the placement of exhaust vents during the leak, but it may be dependent upon their placement after the leak has concluded.

In comparison, the refrigerant concentration dynamics are very different for the $\dot{m}_{low}$ simulation that is illustrated in Figure 2. In this alternate scenario, the refrigerant concentration reaches the RCL only after very long times. It is also clear in considering the comparison of $\overline{C}$ to C_{out} and C_{exh}, in the bottom plot of Figure 3, that there is a noticeable difference between the volume-averaged refrigerant concentration in the room and the local concentrations at the exhaust vent and the undercut. Such a difference indicates a significant amount of stratification for the $\dot{m}_{low}$ case even for $t \leq t_f$ during the refrigerant leak. The higher density of refrigerant causes a correspondingly higher concentration of refrigerant at the bottom of the room, while a lower concentration of refrigerant exists at higher elevations in the room. Such a distribution of refrigerant due to stratification suggests that the undercut must be taken into account when calculating the refrigerant distribution, especially when $\dot{m}_{leak}$ is small, and that the well-mixed assumption will not be valid in such a case.

In comparing the high mass flux leak illustrated in Figure 1 to the low mass flux leak illustrated in Figure 2, it is clear that the the interaction of the downward jet and the room air will result in stratification and a variety of nonuniform spatio-temporal concentration profiles, which depend on $\dot{m_{leak}}$, h_{out} and Q_{exh}. Moreover, the temporally- and spatially-varying nature of the refrigerant flow renders inadequate many of the visual approaches to assessing the amount of stratification, such as scrutiny of the velocity vector field in individual 2-D planes. One measure that can indicate the degree of stratification throughout a space is the buoyancy frequency (Zhang et al., 1996), defined as

$$N^2 = -\frac{g}{\rho_{ref}} \frac{\partial \rho}{\partial z}. \tag{3}$$

The volume average of the density gradient in the direction parallel to the gravitational forces was therefore used in these simulations to compute N^2; the representative buoyancy frequencies for both of the leak rates discussed above are shown Figure 4. This figure is consistent with previous results, in that the larger positive buoyancy frequency after the first part of the initial transient in the $\dot{m}_{low}$ simulation implies that there is a higher degree of stable stratification than in the $\dot{m}_{high}$ simulation. Negative values of N^2 also convey information about unstable density profiles; in the $\dot{m}_{high}$ scenario, the negative value of N^2 for $t > t_f$ implies instability because the ventilation air enters the room and causes an increasing amount of stratification and a "turning over" of the air in the room. This is consistent with results of Figures 1 and 2, in which a difference between the CFD simulations and the well-mixed results is clearly visible for $t > t_f$. The return to higher positive values suggests that the subsequent concentration is again stable, but with a higher degree of stratification.

The effect of varying h_{out} on the refrigerant concentration with constant Q_{exh} was next studied for both $\dot{m}_{high}$ and $\dot{m}_{low}$, as shown in Figures 5 and 6. Two undercut heights of 0.25 inches and 1.2 inches are illustrated in these plots; simulations with intermediate heights were also performed, but were bounded by the cases shown and so only these two simulations are displayed for clarity. There is little visible impact on $\overline{C}$ for $t < t_f$ for the $\dot{m}_{high}$ case, suggesting that the room air is once again well mixed for this period of time. After t_f, however, it is notable that the 1 inch increase in h_{out} results in a large change in the dilution rate. This sensitivity to h_{out} is essentially linear over such heights as might be seen in a door undercut or transfer vent, suggesting that larger values of h_{out} will have a beneficial effect.

In contrast, the value of h_{out} has a much more significant effect on the $\dot{m}_{low}$ scenario of Figure 6. In this case, $\overline{C}$ increases more slowly for the larger value of h_{out} than it does for the smaller value. This can be attributed to a two-layer exchange flow through the wall undercut, in which air enters the room through the wall undercut while the refrigerant leaves the room by a counterflow path (Nabi and

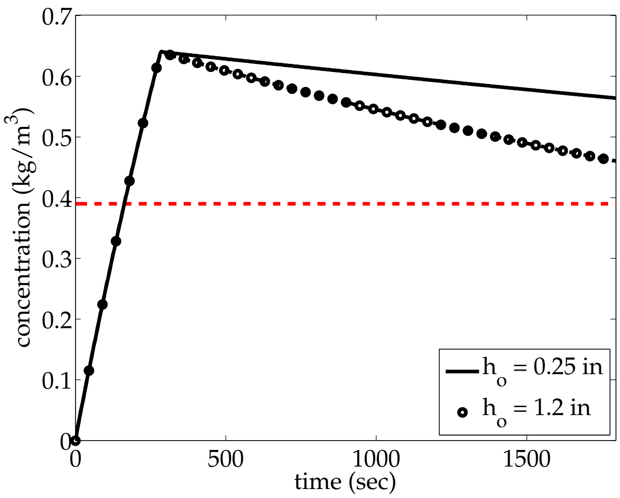

Figure 5: $\overline{C}$ over 1800 seconds during a high-rate leak for cases where h_{out} varies between 0.25 inches and 1.2 inches, with $Q_{exh} = 5$ cfm. The RCL is denoted by the dashed line.

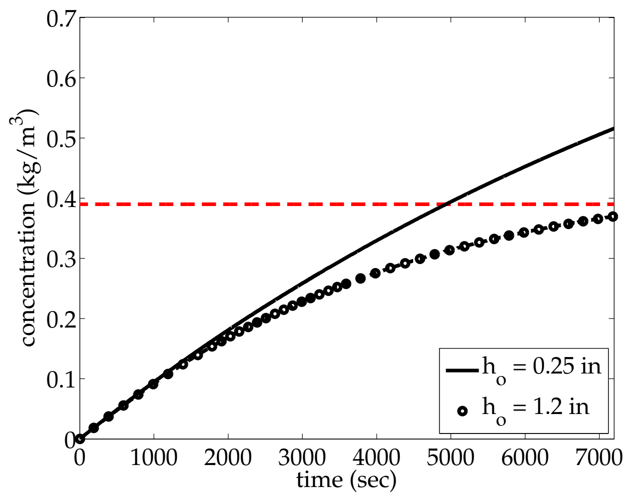

Figure 6: $\overline{C}$ over 7200 seconds during a low-rate leak for cases where h_{out} varies between 0.25 and 1.2 inches, with $Q_{exh} = 5$ cfm. The RCL is denoted by the dashed line.

Flynn, 2013). This exchange flow becomes larger when h_{out} increases. Because this exhange flow rate increases for larger values of h_{out}, the resulting reduction in $\overline{C}$ for the scenario in which $Q_{exh} = 5$cfm and $h_{out} = 1.2$in is sufficient to prevent the refrigerant concentration from exceeding the RCL for the 7200 second duration of the simulation, which accounts for the leakage of the entire 40 pound system charge into the room.

The effect of varying the exhaust ventilation rate Q_{exh} was also studied for both $\dot{m}_{high}$ and $\dot{m}_{low}$, as illustrated in Figures 7 and 8. A variety of simulations were also conducted for different values of Q_{exh} but only the results for exhaust flow rates of 5 cfm and 25 cfm are shown because they bounded the other results. As was the case for the undercut height variation, the $\dot{m}_{high}$ scenario illustrated in Figure 7 exhibits very little variation in $\overline{C}$ during the refrigerant leak $t < t_f$. After t_f, however, the increase of Q_{exh} from 5 to 25 cfm has a significant impact on $\overline{C}$ in the room, causing the refrigerant concentration to return below the RCL after approximately 1200 seconds, or 20 minutes. Such information about the sensitivity of the refrigerant concentration to Q_{exh} could be valuable for a variety of purposes, such as specifying minimum ventilation rates or using the exposure time in tandem with the RCL in the future computation of improved safety factors for Standard 15.

Figure 8 illustrates what is perhaps the most surprising and encouraging result observed in this research, which is that it is possible to leak 40 pounds of refrigerant into this small space while approaching an asymptote below the RCL. For the modest parameter values of $\dot{m}_{low} = 2$ g/s prescribed by ISO 5149-3, $h_{out} = 0.25$ in, and $Q_{exh} = 25$ cfm, the refrigerant concentration hits a peak of 0.2 kg/m^3, which is only about half of the RCL. The stratified nature of the concentration field is responsible for this phenomenon, as the exchange flow through the wall undercut and the exhaust vent are able to effectively remove room air with a relatively high concentration of refrigerant. Such results are particularly exciting, because they raise the possibility of designing HVAC&R systems which are inherently safe, as long as a set of design assumptions are met on leakage rates and room conditions, without resorting to the present conservative restrictions on total system charge.

The importance and potential advantages of using this stratification are further emphasized by the

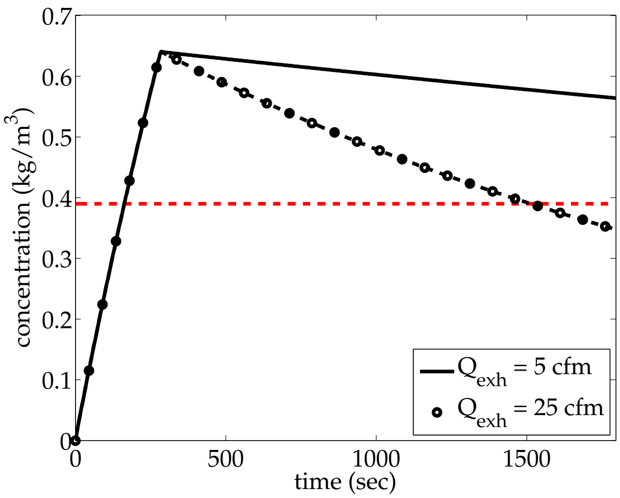

Figure 7: $\overline{C}$ over 1800 seconds during a high-rate leak for cases where Q_{exh} varies between 5 cfm and 25 cfm, with $h_{out} = 0.25$ in. The RCL is denoted by the dashed line.

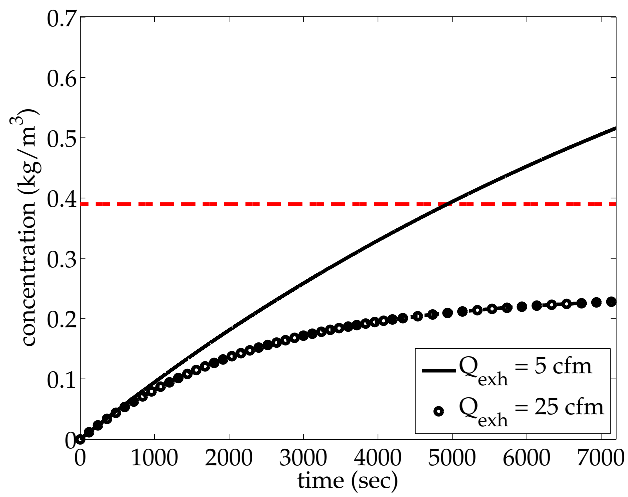

Figure 8: $\overline{C}$ over 7200 seconds during a low-rate leak for cases where h_{out} varies between 0.25 and 1.2 inches, with $Q_{exh} = 5$ cfm. The RCL is denoted by the dashed line.

simulations illustrated in Figure 9. This figure illustrates $\overline{C}$ for three related scenarios: one in which the refrigerant leak is located in the middle of the ceiling and the exhaust vent is located in the top corner of the room (black line), one in which the exhaust vent remains in the same location but the refrigerant leak is moved to the middle of the wall above the undercut (green line with circles), and one in which the refrigerant leak is located in the middle of the wall but the exhaust vent is moved to a location two feet above the floor on the opposite wall (blue line with squares). Identical values of $\dot{m}_{low}$, Q_{exh}, and h_{out} were used in all three of these simulations. The extent to which the concentration field is sensitive to geometric parameters is abundantly clear from Figure 9; the low height of the exhaust vent for the third simulation enables it to remove air with a high concentration of refrigerant, while the high height of the exhaust vent in the second simulation, coupled with its increased distance from the refrigerant leak, makes it less effective than the baseline case.

4 Model-Order Reduction Methods

Over the last two decades, a new Lagrangian flow analysis technique has been developed to study unsteady fluid phenomena. This involves the computation of so-called Lagrangian Coherent Structures (LCS) (Haller, 2001), which are time-varying boundaries of dynamically distinct regions of the flow. These structures are particularly interesting because there is near-minimal flux across their boundaries between the different regions over the time horizon on which they are computed. These structures are usually computed as ridges of the leading finite-time Lyapunov exponent (FTLE), which is a scalar field proportional to the maximal exponential rate of growth of material lines over the time horizon of computation (Shadden et al., 2005). Figure 10 illustrates an isosurface for the forward time FTLE. This FTLE clearly captures the structure of the downward jet, and also shows that there is unmixed region near the near injection site. Because the streamlines of a transient flow field give no useful information about the fate of fluid particles over any significant time horizon, LCS is an appropriate analysis tool for delineating important Lagrangian structures that govern the flow in the room for different operating

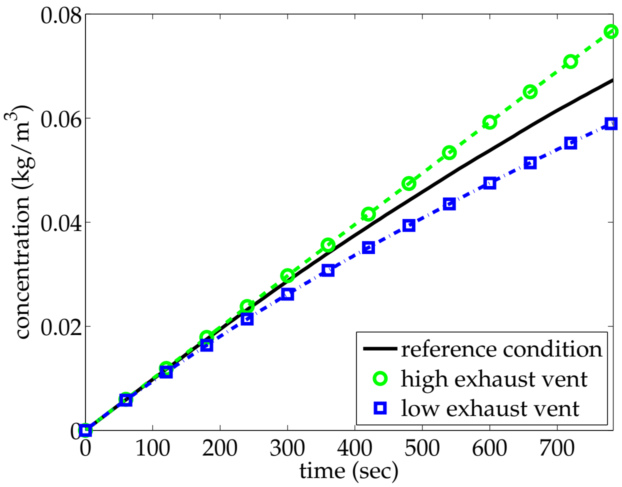

Figure 9: $\overline{C}$ for different locations of exhaust vent and refrigerant injection.

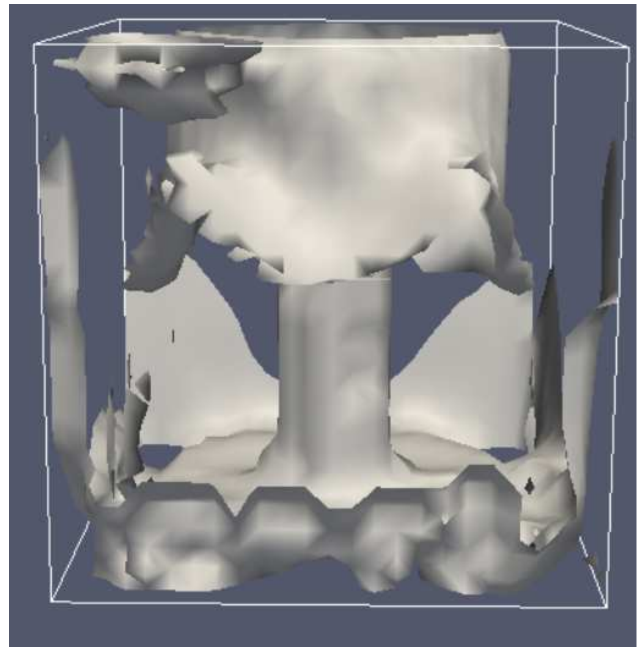

Figure 10: Isosurface for the forward time FTLE.

and leakage parameters. This analysis is especially useful in the cases where well-mixed assumption is known to be violated, such as is the case in the refrigerant dispersion context discussed in this paper. Such early results using LCS for analysis of refrigerant and air flow in rooms have been encouraging, and will be the topic of future research and publications.

5 Conclusions and Future Work

The dispersion of refrigerant in occupied spaces is a complex phenomenon, due to the presence of many spatial and temporal scales. Different fidelity models of refrigerant leakage scenarios can lead to very different conclusions, depending on the relevance of the assumptions involved in modeling. In particular, the well-mixed assumption is not a useful assumption for low-rate refrigerant leakage. The specific geometric configuration of the low-rate leakage can actually result in cases where the refrigerant never exceeds the RCL, which is somewhat remarkable. Using a combination of CFD, low order models and experiments will hopefully help us to improve Standard 15 and facilitate both innovation and the safety of room occupants for the next 100 years.

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