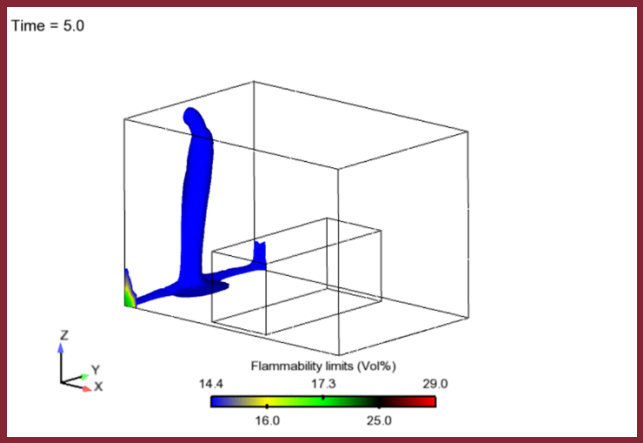


A Novel Simulation-based Fire Risk Hazard Ranking for Refrigerant Leakage in Confined Spaces

Sangamesh Hosur
Mahmood Tabaddor, PhD

RESEARCH REPORT
(DISTRIBUTION: EXTERNAL/PUBLIC)
NOVEMBER 2018

UL LLC
333 Pfingsten Road, Northbrook, IL 60062-2096 USA
www.UL.com

DISCLAIMER

This report was prepared for research purposes only by UL staff. The information contained herein relates only to the products tested for the purposes of this report. UL LLC does not warrant that this information is complete or accurate or is applicable to products other than those actually tested. This report does not mean that any product referenced herein is Listed, Classified, Recognized or otherwise certified by UL, nor does it authorize the use of any UL certification marks or the UL name or logo in connection with the product or system. In no event shall UL LLC, or its be liable for any damages, loss, claims, costs, or expenses arising out of or resulting from the reliance on, use, or inability to use the information contained herein. Nor shall UL LLC, or its affiliates be liable for any errors or omissions in the report.

TABLE OF CONTENTS

ABSTRACT

In this paper, we present a new risk metric to measure the probability of fire when there is leakage of a combustible refrigerant gas into a confined space. This risk metric can only be obtained via computational fluid dynamics modeling (CFD) software such as OpenFOAM. In essence, we track the volume of combustible gas that lies between the upper and lower flammability limits. We demonstrate how the risk metric can change depend upon a change in the details of the leakage scenario.

Keywords: *OpenFOAM, Species transport, turbulence, refrigerant leakage, diffusion, fire risk*

INTRODUCTION

An overall effort to reduce the greenhouse warming potential of refrigerants for refrigeration systems has reduced the overall candidate list to refrigerants that exhibit higher flammability than their predecessors. This has required investigations to ensure that the potential fire/explosion hazards associated with leakage of a flammable refrigerant are properly addressed and mitigated. The main means to gaining this understanding has been through physical testing [1].

However, there is a challenge and a limit to using physical testing to thoroughly understand the potential risks associated with leakage of a combustible refrigerant in confined spaces. The challenge is that physical testing, especially if it could involve fire and explosion, is expensive and time consuming. Each test is a single data point and so many tests must be run which requires significant funding. Yet, it is another limit of physical testing that is most problematic. It is only possible to capture data at discreet points in physical testing. These discrete points are usually selected to address the specific question the test was designed to answer and so the data collected may not provide sufficient insight into the testing conditions or allow for generalization.

An alternative to physical testing, or rather a complement, is the use of computational modeling tools. These tools have been used sporadically to help understand the risks associated with leakage of combustible refrigerants[2,3]. For modeling, the key challenge is to validate the simulation, that is to demonstrate via experimental evidence that the model predictions are accurate [4,5,6]. In one research report [1], the results of testing and simulation were compared yet the validation of the simulation was not properly conducted. In other similar research conducted on refrigerant leakage hazard, the published reports [2,3] demonstrated good agreement between the model predictions and those from the test, and yet only a single point was selected for this conclusion. This is not sufficient to establish high confidence validation and could potentially hide flaws in the model that become more prevalent when used for other leakage scenarios.

Finally, there is a challenge of using a few discrete points to assess the fire/explosion risk of a particular combustible refrigerant leakage scenario. When the intent is to determine if ignition of the leaked refrigerant is possible, the exact location of the ignition sources are critical and ignition outcomes could change drastically depending on the location of the ignition source(s) and local gas concentration levels. Also, the risk scenario of an active combustible gas leak is time dependent and therefore, a single fire or no fire outcome from an ignition source activated at a particular instant of time is not sufficiently informative of the full transient state.

The intent of our research is to demonstrate two things: (1) rigorous validation evidence for a simulation of refrigerant leakage in gaseous form in a confined space. And, (2) a new risk metric for assessing the fire/explosion hazards associated with leakage of refrigerant into a confined space. This metric can only be obtained from the rich data provided by such computer-based engineering tools. Item 1 has been covered in a paper titled Refrigerant gas leakage in ISO room: A comparative computational fluid dynamics (CFD) study to be published [7]. In this paper, we will focus mainly on item (2).

Overall Approach

To demonstrate our approach, we built a model intended to replicate results seen during refrigerant leakage testing conducted at UL for an AHRI funded project [8]. We selected one room type along with different factors allowing for different leakage scenarios. We will describe some aspects of the CFD model though more detail which is available in another paper [7]. Then we will define the new fire risk metric for the different scenarios and show its usefulness for risk assessment.

TEST SET-UP

The test that was simulated was carried out at the fire testing facilities at UL [8]. A 3.6 m by 2.4 m by 2.4 m room was constructed within the facility as shown in Figure 1. A room was constructed with dimensions in accordance with ISO 9705 [9]. The room contained an obstruction (representing a couch) of 1.83 m by 0.91 m by 0.91 m size at the center of the room. The room was equipped with refrigerant sensors at select locations to measure the leakage of R32 gas concentrations. The refrigerant was leaked in a gaseous form in a controlled fashion with test parameters being leakage location and leakage rate. Ignition sources were placed at one location in the room where a spark was generated at a specified point in time. Further details about the experiment can be found in the UL report [8].

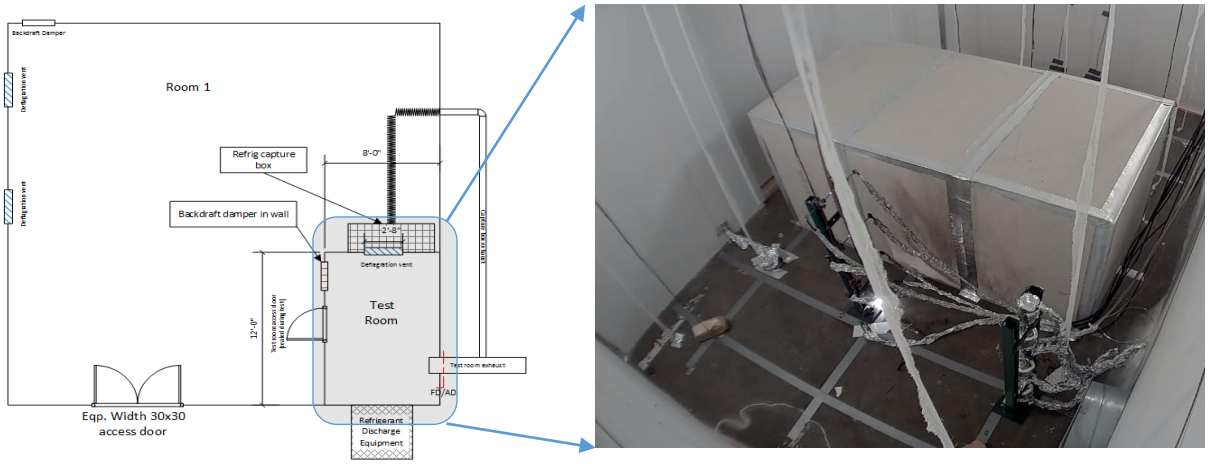


Figure 1 *Test room schematic (left) picture of inside of test room (right)*

CFD SIMULATION

The model for refrigerant gas leakage for the testing scenarios described in previous section was developed using OpenFOAM, an open source CFD code [10]. CFD analysis was carried out to investigate the influence of refrigerant release rate and location on the spatial and temporal refrigerant concentration levels in a test room scenario described in previous section. The simulation provides predictions of the gas concentrations throughout the room for each scenario. The kcy challenge is to properly capture the physics of turbulence, diffusion and buoyancy which help determine the concentration gradient within the room. For the purposes of this research, we do not model the actual combustion process[1] as the focus for this simulation is on the gas concentration levels within the room. By monitoring the gas concentration levels throughout the room and over time, we can then compare those values to the upper and lower flammability limits for the refrigerant gas to determine propensity for fire should an ignition source exist. More on this in the results section.

1.1 Physics of Flow

The refrigerant gas leakage was modelled using the solver rhoReactingBuoyantFoam in OpenFOAM toolbox[12]. It is a solver for combustion with chemical reactions using a density based thermodynamics package with enhanced buoyancy treatment. The solver was initially developed for reacting flows, the chemical reaction source term in the chemical species conservation equation was disabled as there will be no reaction (combustion) between air and refrigerant namely R32 for our purposes. In order to capture gas diffusion phenomenon solver uses the effective viscosity for species diffusion which is shown in the code below. In this code muEff is defined as muEff = mu( ) + mut( ). The first term mu( ) is defined as constant in the transport properties where as mut( ) is initialized with a value 0 but this is calculated based on the turbulence model included in the set up and values are updated for every iteration. A portion of the code capturing the detail is shown next.

```
fvScalarMatrix YiEqn
    (fvm::ddt(rho, Yi)
     + mvConvection->fvmDiv(phi, Yi)
     - fvm::laplacian(turbulence->muEff(), Yi) == reaction->R(Yi)
     + fvOptions(rho, Yi) );
```

The chemical properties in the chemistryProperties file located in constant directory was set to inert. Hence solver covers species transport simulation with R32 being a single species. This solves mass, momentum and energy equations along with a species transport equation [12,13,14].

A species transport equation is shown in (1). It describes convection and diffusion for the species *i* for an unsteady condition without reaction [15] [16].

$$\frac{\partial(\rho\ \mathrm{Yi})}{\partial t} + \nabla.(\rho\ \mathrm{U}\ \mathrm{Yi}) = -\nabla.(\mathrm{Ji}) + Si \qquad (1)$$

[1] The intent of the safety standard is to mitigate the possibility of a flammable concentration level near an ignition source.

Here ρ is the density of species i, Yi is the mass fraction of species i, U is the three dimensional velocity components, t is time, Ji is the diffusion flux of species i and Si is the source term of species i. The convection term div(ρ*U*Yi) is transport material due to velocity of the fluid. Diffusion div(Ji) represents the transport term resulting from concentration gradients.

The mass diffusion due to the mixing action of the chaotic turbulent velocity fluctuations is given as

$$Ji = -\rho \, \mathrm{Di} \, \nabla(\mathrm{Yi}) - (\mu t \, / \, \mathrm{Sc}) \, \nabla(\mathrm{Yi}) \tag{2}$$

Here μt is the turbulent viscosity and Sc is the turbulent Schmidt number. The reaction term was neglected as the concern is only with the air-refrigerant mixing behavior.

Fluid Properties

The fluid properties considered for simulation in accordance with test set up are shown in the Table 1.

Table 1 *Thermo-physical Fluid properties*

Fluid Property	Air	R32
Molecular weight	29	52
Density (kg/m^3)	1.225	2.214
Kinematic viscosity (N s/m^2)	1.789e-05	1.155e-05
Thermal conductivity (W/mK)	0.0242	0.0124
Prandtl No	0.75	0.833
Specific heat Cp (J/K)	1006	830.2

Geometry

The ISO 9705 room defined the computational domain and is shown in Figure 2. The room was modified to include three inlets which are located at 0.2 m, 1.8 m and 2.2 m height from the floor on one wall opposite to a door. Each inlet allowed for controlled leakage of the refrigerant gas. The flow conditions for the AHRI 9007 project[8] was designed to simulate a constant mass release at expected temperature/pressure conditions at a leak point in the subcooled liquid line. The fact that it would release as a gaseous form was ancillary. During each test, only a single inlet was activated. A 3 mm gap between the door and floor was included in the model with the length of the gap being 0.9 m. The obstacle in the middle of the room, representing furniture, was also included as its expected impact on air flow is substantial.

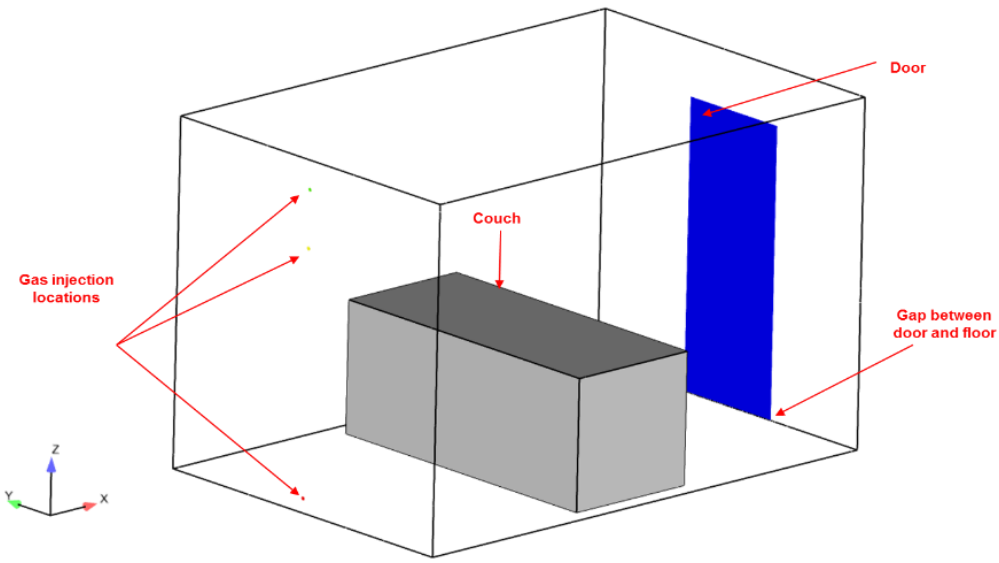


Figure 2 *Geometric model of test room*

Meshing

The entire computational domain was meshed using Hex elements employing ANSYS ICEMCFD [11]. A mesh dependency study was carried out with two different mesh sizes as shown in Figure 3. An analysis of the results show that the difference between the coarser and finer meshes were marginal as shown in Figure 4. Hence the coarser mesh was selected for its computational efficiency for all subsequent results in this report.

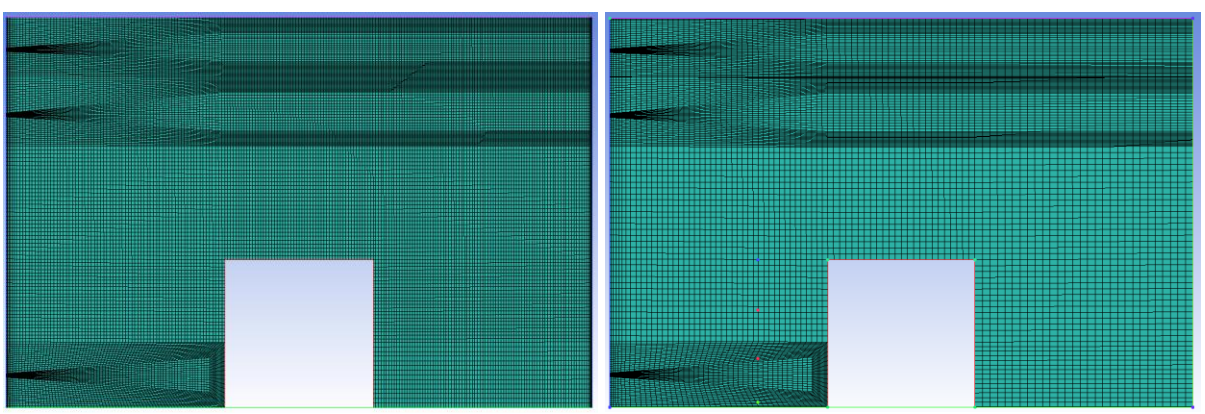


Figure 3 : *(left) coarse mesh with 0.6 million cells (right) Fine mesh with 1.2 million cells*

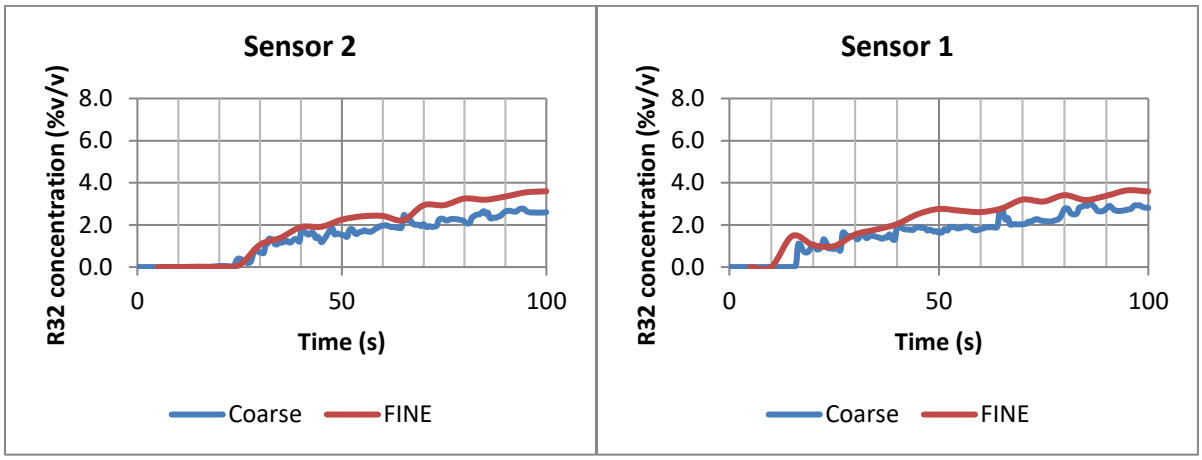


Figure 4 *Mesh sensitivity study*

Scenarios

For this study, six different refrigerant gas leakage scenarios were studied. The factors under consideration were the gas leakage rate and the location (height) of the leak. The opening size was kept constant. Actual test times varied as the objective of these tests was to introduce a fixed mass of gas (3.25 kg) for all scenarios. All six cases are summarized in Table 2.

Table 2 *Case studies for risk analysis*

Scenario No	Release Rate (g/s)	Release Height (m)	Simulation Time (s)	Opening Size in mm
1	13.5	2.2	240	25
2	13.5	0.2	240	25
3	50	2.2	67	25
4	50	0.2	67	25
5	100	2.2	33.5	25
6	100	0.2	33.5	25

RISK METRIC

When a combustible gas is released into a confined space where an ignition source could be present, there is a possibility of a fire and/or explosion taking place. Part of the risk is determined by the gas concentration levels. For combustion of gases, the concentration level must reside within an interval defined by the lower and upper flammability limits [17]. The upper and lower flammability limits for the refrigerant in this study, R32, are 14.4% and 29.3% by volume, respectively [18]. The power of computer simulation is that we can measure and track the size and location of the what we are calling the Flammability Volume (FV) of the leaked gas. The FV is the volume of leaked gas that is between the upper and lower flammability limits. This will not only contribute to the probability of a fire, but also to predict the magnitude of an event. By tracking the size and location of the Flammability Volume and normalizing it by the volume of the room, we define a new risk measure called Normalized Flammability Volume (NFV) which represents the probability of a fire/explosion occurring assuming the ignition sources are randomly distributed in the entire room. Values of NFV will reside between 0 and 1 with 1 being a certain occurrence of fire/explosion in the presence of an ignition source since the FV occupies the entire volume of interest in the compartment.

Of course, it is possible that the ignition sources are not distributed throughout the room but within a smaller fraction of the room. In that the case, the Flammability Volume is normalized by a portion of the volume of the entire room, called the volume of interest (VOI), where the ignition sources are most likely to reside. The values of NFV still reside between 0 and 1 with a higher value suggestive of a higher probability and risk of fire/explosion. So more generally,

$$\mathrm{NFV} = \mathrm{FV}\ (\textit{in VOI})/\ \mathrm{VOI} \qquad (3)$$

Next we examine how the NFV approach provides insights into the fire risks of the different scenarios shown in Table 2. As can be seen in Figure 5, the different scenarios were not all run for the same length of time, since as described earlier, the test times were not the same. This is because the total amount of refrigerant introduced in the room was the fixed for each scenario and so depending upon the flow rate, the time of each test varied.

Now looking at close up of the data, Figure 6, some trends for NFV can be seen. During the initial stages of the gas leakage the NFV is indistinguishable amongst most of the scenarios, however, at the 15 second mark, the NFV for Scenario 6 starts to build up quickly followed by Scenario 2 and then Scenario 4. Scenario 6 is stopped earlier than the other two scenarios as it reached the target amount of total refrigerant to be introduced. Note that all 3 of these scenarios share the single feature that the leakage occurs at the lowest level within the room. In these cases, the presence of the floor and the obstacle in the middle of room are likely creating constraints on the flow that allow for a quicker buildup of the leaked gas concentration levels exceeding the lower flammability limit.

Scenario 5, where the gas leaked from a top location in the room appears to match, up to 15 seconds, the concentration levels of NFV with the three scenarios just discussed. However, it is does display a growth rate that more closely matches Scenarios 3 and 1 as the simulation was run longer for Scenario 5. For the scenarios where the leak is at a high location in the room, the rate of growth of NFV is steady but very slow. This is likely due to the fact that once the gas leaks it can begin to move downward towards the floor due to buoyancy forces. Build up behavior of the NFV over time is basically linear for the highest leak location versus an exponential type rise for the lower leak location. This already shows the risk profile changes simply based on location of the leak.

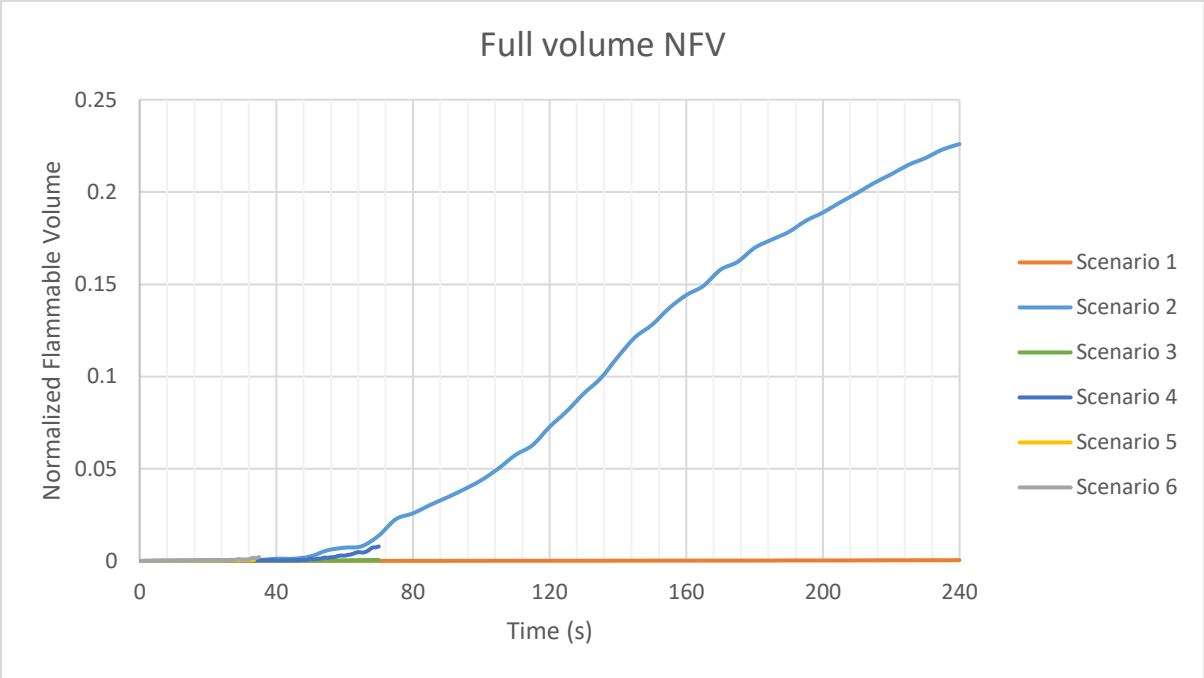


Figure 5 *NFV normalized to full room volume*

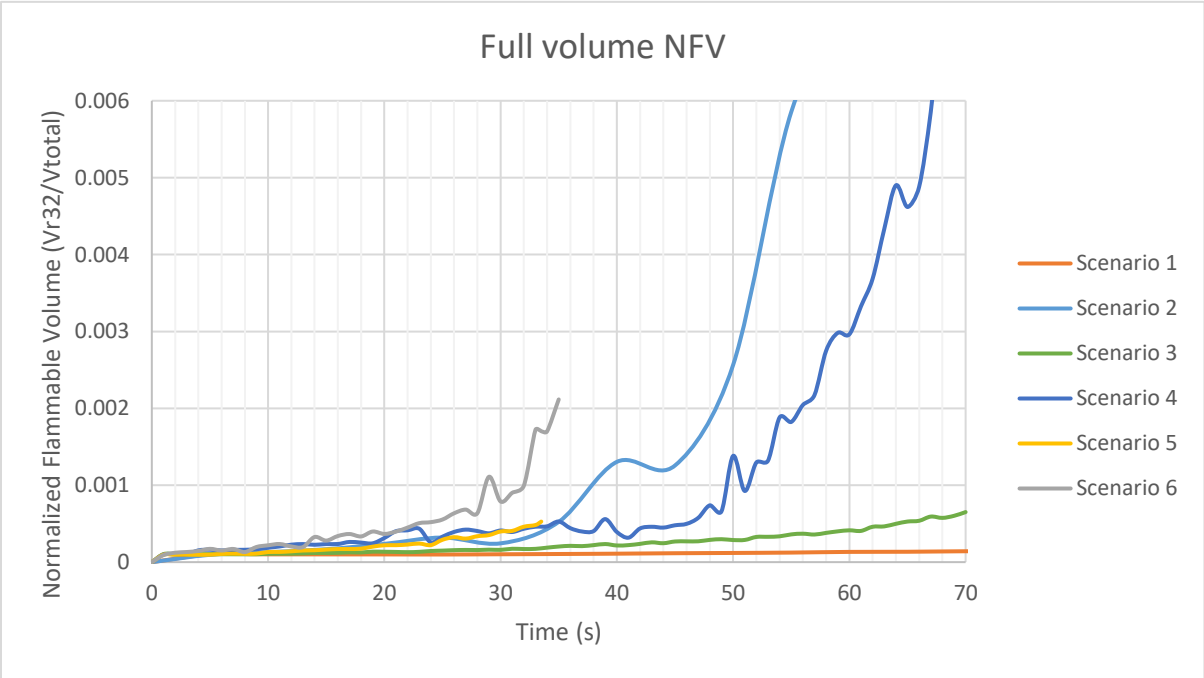


Figure 6 *Close up of Figure 5*

Next we compare the NFV for the same scenarios but normalized with respect to the bottom half of the room. One reason a select portion of the room may be important is that it is the main region where ignition sources exist [8]. Also note that the FV changes as now only portion of the FV that resides in the VOI which is the lower half of the room. Figure 7 shows the NFV for this reduced portion of the room.

For the new VOI, the same three scenarios, with leakage from the bottom of the room, lead to highest values of NFV. In the same order, Scenario 6 exhibits the highest value of NFV, followed by Scenario 2 and finally Scenario 4. Note that Scenario 5 results in a negligible NFV. In other words, when the VOI is reduced to the bottom half of the room, the magnitude of the NFV increases for the scenarios where the leak is near the bottom of the room. Whereas, for the scenarios where the leak occurs near the top of the room, the NFV risk falls to zero. This analysis gives a more refined insight in that if the ignition sources are known to reside in a specific volume then it might be more relevant to reduce the size of the normalization volume as much as possible to get more exact value of NFV.

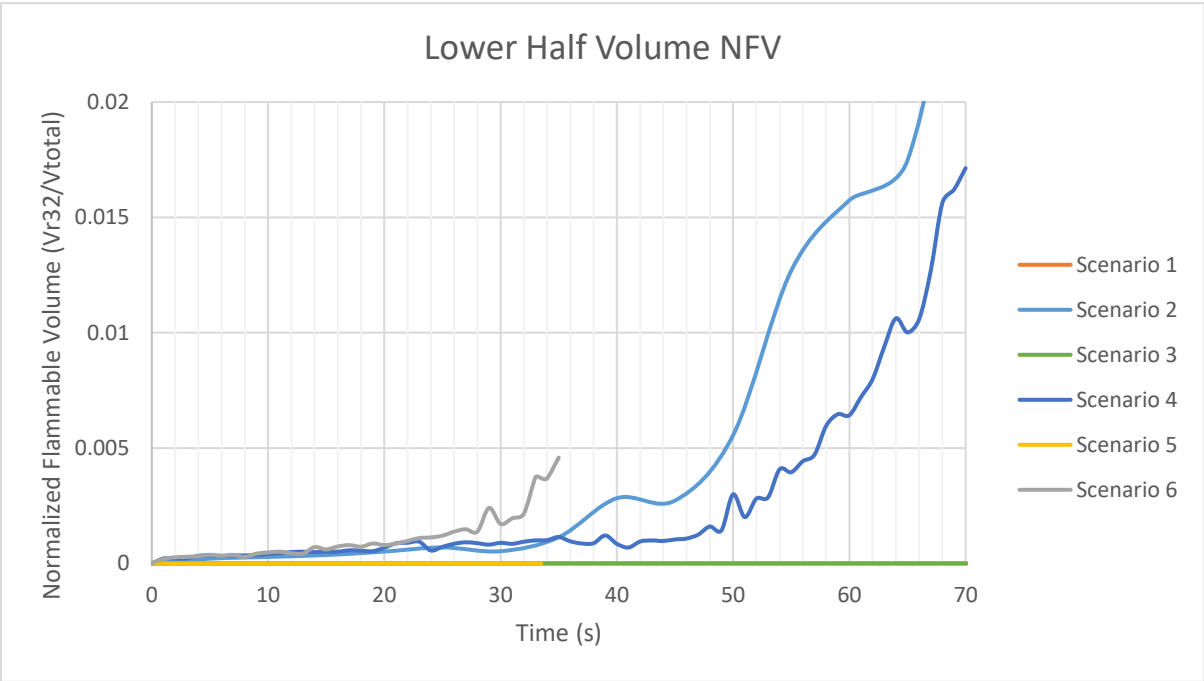
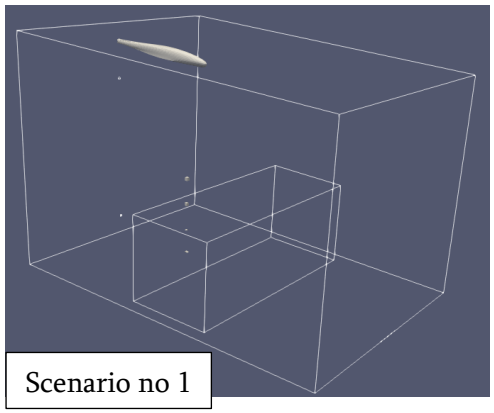
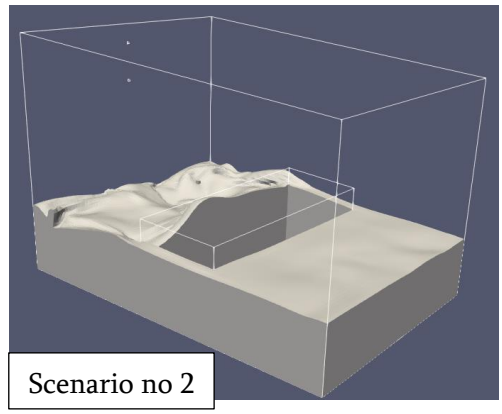
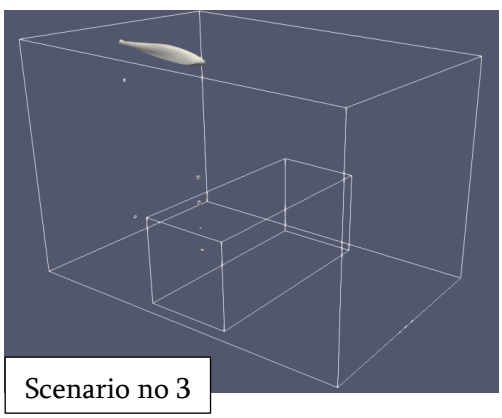
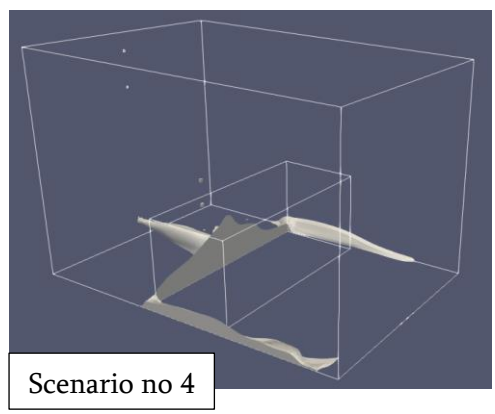
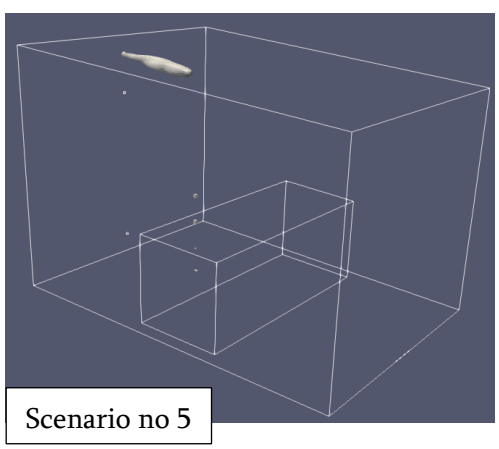
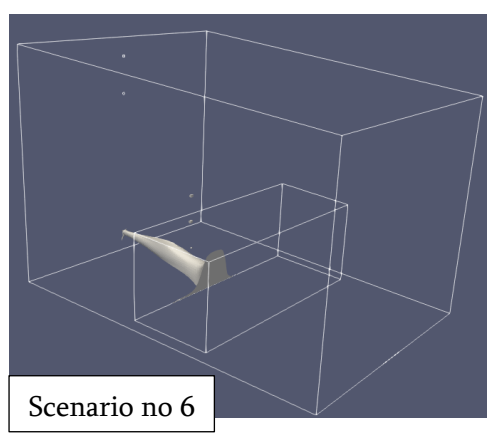


Figure 7 *Closeup of NFV normalized to volume of lower half of room*

Finally, we demonstrate another strength of the CFD and that is visualization of the FV. The FV of these scenarios at the time when the test was stopped (just before ignition) is shown in Table 3. The visualization of FV using an iso-volume helps investigators and designers see the size, shape and location of the FV. In scenario 6, it was observed that about 25% of total room volume was completely occupied with FV. Three ignition sources (from the test setup) are completely located inside the FV. In scenario 2 and 4, FV is restricted to the floor level between the inlet and the couch. It was also observed that only lower ignition

source near floor was submerged. But in scenario 1, 3 and 5, FV is only located near the top inlet zone which was far away from all ignition sources. One other interesting insight is that in all cases the FV was a single volume, this is not expected to be a result that can be generalized to any scenario. There could be scenarios where instead of a single FV there may be multiple FV within the same confined space. However, the NFV calculation is not predicated on the FV being continuous.

Table 3 *Flammable Volume of R32 for different scenarios at time of ignition in test*

	TOP	BOTTOM
13.5gps at 240s	 Scenario no 1	 Scenario no 2
50gps at 67s	 Scenario no 3	 Scenario no 4
100gps at 33.5s	 Scenario no 5	 Scenario no 6

CONCLUSION

In this paper, we have introduced a new risk metric, normalized flammability volume (NFV), one that represents the probability of fire/explosion during refrigerant gas leakage into a confined space. We have also demonstrated its value using a specific room scenario that was part of a physical test investigation. The power of this metric is that it can track the changing nature of the risk (probability of fire) during a leakage event when combustible gas is being introduced into a confined space. The gas concentration levels are determined by the physics of the flow and details of the room. We discuss how the risk metric can help rank different scenarios. This risk metric is not available from physical testing and can only be obtained from high fidelity and validated CFD models.

ACKNOWLEDGMENTS

The authors would like to acknowledge the technical support for OpenFOAM by Mohsen Battoie from ESI Group. The authors would also like to thank George Hunter and Mark Skierkiewicz from UL LLC.

REFERENCES

[1] "AHRI Project 8009 Final Report : Risk Assessment of Refrigeration Systems Using A2L Flammable Refrigerants" Gradient Corp report 2015

[2] "AHRI Project No. 8016: Risk Assessment of Class 2L Refrigerants in Commercial Rooftop Units" Navigant corp report 2016.

[3] "AHRI Project 8004 Final Report Risk Assessment of Residential Heat Pump Systems Using 2L Flammable Refrigerants" Gradient Corp report 2012

[4] Lizhi Jiaa, Wufeng Jina, and Yan Zhangb "Analysis of Indoor Environment Safety with R32 Leaking From a Running Air Conditioner" 9th International Symposium on Heating, Ventilation and Air Conditioning (ISHVAC) and the 3rd International Conference on Building Energy and Environment (COBEE)

[5] Safety research of A2L/A3 refrigerants and risk assessment in japan by Eiji Hihara

https://www.jraia.or.jp/english/side/presentation3.pdf (Accessed 04th Oct 2018)

[6] https://www.grc.nasa.gov/www/wind/valid/tutorial/valassess.html (Accessed 04th Oct 2018)

[7] Sangamesh Hosur, Sachinkumar Rai, Mahmood Tabaddor "Refrigerant gas leakage in ISO room: A Comparative CFD Study" Presented at NAFEMS India Regional Conference on Engineering Modelling, Analysis, Simulation and 3D-Printing (NIRC-2018) 20 – 21 July 2018, Bengaluru, Karnataka, India.

[8] AHRTI Report No. 9007-01, Benchmarking risk by whole room scale leaks and ignitions testing of A2L refrigerants, UL Research Report, 2017.

[9] ISO 9705-1: Reaction to fire tests - Room corner test for wall and ceiling lining products - Part 1: Test method for a small room configuration - First Edition

[10] https://www.openfoam.com/ (Accessed 04th Oct 2018)

[11] https://www.ansys.com/en-in/services/training-center/platform/introduction-to-ansys-icem-cfd (Accessed 04th Oct 2018)

[12] Juliane Fiates, Sávio S.V. Vianna "Numerical modelling of gas dispersion usingOpenFOAM", Journal of Process Safety and Environmental Protection, 1 0 4 (2 0 1 6) 277–293.

[13] A. Mack∗, M.P.N. Spruijt "Validation of OpenFoam for heavy gas dispersion applications" Journal of Hazardous Materials 262 (2013) 504– 516

[14] Longxiang Dong, Hongchao Zuo*, Liang Hu, Bin Yang, Licheng Li, Liyang Wu, "Simulation of heavy gas dispersion in a large indoor space using CFD model" Journal of Loss Prevention in the Process Industries 46 (2017) 1e12

[15] H. K. Versteeg and W. Malalasekera, An introduction to computational fluid dynamics: The finite volume method, 2 ed. Harlow, England: Pearson Education, 2007.

[16] Christoper J. Greenshields and CFD Direct Ltd. (2015). OpenFOAM, The Open Source CFD toolbox, User Guide , Version 3.0.1.

[17] Quanyi Liua, Hui Zhanga , Yi Liua , Hong Huanga , Xiaole Zhanga , Zhipeng Lib , Wei Yaoa "Influencing factors of flammable refrigerants leaking in building airconditioning System" The 9th Asia-Oceania Symposium on Fire Science and Technology, Procedia Engineering 62 (2013) 648 – 654.

[18] "Safety data sheet" by National Refrigerants.Inc http://www.refrigerants.com/pdf/SDS%20R32.pdf (accessed 05th Oct 2018)