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Milestone Report BTO 3.2.2.25 – Methodology for Estimating Safe Charge Limits of Flammable Refrigerants in HVAC&R Applications – Part 1

Van Baxter
Omar Abdelaziz
Ahmad Abu-Heiba
Dean Edwards
Ahmed Elatar
Charles Finney
Viral K. Patel
Mingkan Zhang

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OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

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Energy and Transportation Sciences Division

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Van Baxter
Omar Abdelaziz
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Mingkan Zhang

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OAK RIDGE NATIONAL LABORATORY
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EXECUTIVE SUMMARY

Refrigerant flammability introduces new challenges to the usage of low global warming potential (Low GWP) refrigerants in real life applications. Those challenges are centered around the deflagration risk associated with their use and its implications on personal safety. Standards have been developed to systematically set maximum allowable flammable refrigerant charges to ensure safety in case of refrigerant leakage. These standards were initially based on limited testing and numerical analyses of refrigerant leakage into confined spaces. Currently published general safety standards include International Standards Organization (ISO) 5149, and its relative counterpart ANSI/ ASHRAE 15

Equipment standards include the International Electrotechnical Commission (IEC) standard suite, IEC 60335-2-24, IEC 60335-2-40 and IEC 60335-2-89. The corresponding CANENA standards are Underwriter's Laboratories (UL) UL 60335-2-24, UL 60335-2-40 and UL 60335-2-89, along with UL 471, UL 563, etc.

These standards were developed based on non-flammable and flammable refrigerant categories. Flammable refrigerants have been included in the IEC and ISO standards for over two decades and have been included more recently in the North American standards. The cognizant bodies for these standards are engaged in revision/update processes. A main objective of current revision work is to include requirements for the "A2L refrigerant" category in ANSI/ASHRAE 34 and ISO 817 standards.

Most low GWP refrigerant options are either class A2L (lower flammability) or A3 (higher flammability). To enable the deployment of environmentally friendly Low GWP refrigerants, the standards and codes working groups must have reliable, publicly available, science-based data and information to safely use these refrigerants. Information is needed to enable credible safe charge limit estimates for the different flammable refrigerant options for various heating, ventilation, air-conditioning and refrigeration (HVAC&R) applications. Currently, there are gaps in the required information. The goal of this project, Flammable Charge Limits Estimation project, are to 1) prioritize the required information, 3) identify information gaps and 3) fill them in to the extent possible within limits of the project resources.

This is the first of two planned reports for this project.

Report 1: *Methodology for Estimating Safe Charge Limits of Flammable Refrigerants in HVAC&R Applications – Part I.*

This volume provides an overall summary of the project approach and tasks. Summaries of the initial stakeholders' workshop, prior literature and research survey, and the computational fluid dynamics (CFD) modeling approach, calibration and validation, and testing are presented. Simulations of a 4-room single-family home and duct system are presented along with summary results and concluding observations. Several refrigerant leak case simulations and results for small room ACs are discussed as well.

Report 2: *Methodology for Estimating Safe Charge Limits of Flammable Refrigerants in HVAC&R Applications – Part II.*

This volume will provide a summary of the development of reduced order models (ROM) for estimation of safe charge limits based on a computational fluid dynamics (CFD) parametric study. The study focus is on refrigerant releases in a single room for a range of parameters including refrigerant, refrigerant release rate, quantity and height, outdoor air ventilation rate, and room floor area. Two ROM versions are planned: one with no room air circulation (air conditioner blower off) and one with circulation.

E.1 WORKSHOP

ORNL held a workshop on October 24th of 2016 to solicit critical input from stakeholders in industry and other organizations to help guide the project and achieve results most useful to the US HVAC&R and Appliances community. ASHRAE hosted the workshop at its Atlanta Headquarters Offices. The top four priority CFD case study recommendations that emerged from the workshop are listed in Table E.1, below.

Table E.1. Ideas and Suggestions from Case Studies Session

Idea/suggestion	Votes
Room that meets minimum floor area requirements for m_2	13
Leak profiles in various applications of RTU, mini split and VRF units	10
Validate the underlying premise of the standard for m_1, m_2 and m_3	5
Residential split heat pump air handler unit in utility closet	2

E.2 LITERATURE REVIEW

A review of the literature was conducted including previous analytical and experimental studies of leak events, probabilistic risk assessment (PRA) studies, international guides and resources, and relevant safety standards dealing with flammable refrigerants.

International standards and refrigerant safety classification standards from ANSI/ASHRAE, ISO, and IEC provide information about permissible locations for systems employing flammable refrigerants, corresponding maximum quantities of refrigerant charge, construction requirements for the mechanical systems and external features associated with installation, such as ventilation and detection. The standard which is most relevant to the current work is IEC 60335-2-40. The US Underwriters Laboratories (UL) embodiment of IEC 60335-2-40 is called UL 60335-2-40. Below is a list of the main issues impacting flammable refrigerant usage in IEC 60335-2-40:

1. Flammable refrigerant charge limits and equations were initially developed for A3 and A2 refrigerants. Standard revision proposals to allow higher charge limits for A2L refrigerants should be verified for safe use.
2. Conservative failure conditions were used during the standard development: low leak velocity, fixed 4 min leak rate, downward leak direction, tight room, no ventilation, no oil presence, no air flow.
   These conditions may prove to be overly restrictive for newer A2L refrigerants which have relatively high minimum ignition energy and low burning velocity, especially if sufficient mitigation is present.
3. Presence/absence of obstacles (e.g., room furnishings, etc.) on refrigeration dispersion during release events is also not well understood.

Many experimental and numerical studies were found in the literature for both A2L and A3 refrigerant leaks. For most studies reviewed, there was no clear connection to the maximum charge limits prescribed by the pertinent standards. A summary of a small sample of the studies is depicted in Figure E.1. These illustrate the relationship between flammable refrigerant charge limits (m_{max}, according to IEC 60332-2-

40), actual charge, (m_c) maximum concentration (c_{max}) and LFL. The details of the simple analysis used to generate Figure E.1 are given in Section 3.2.1.

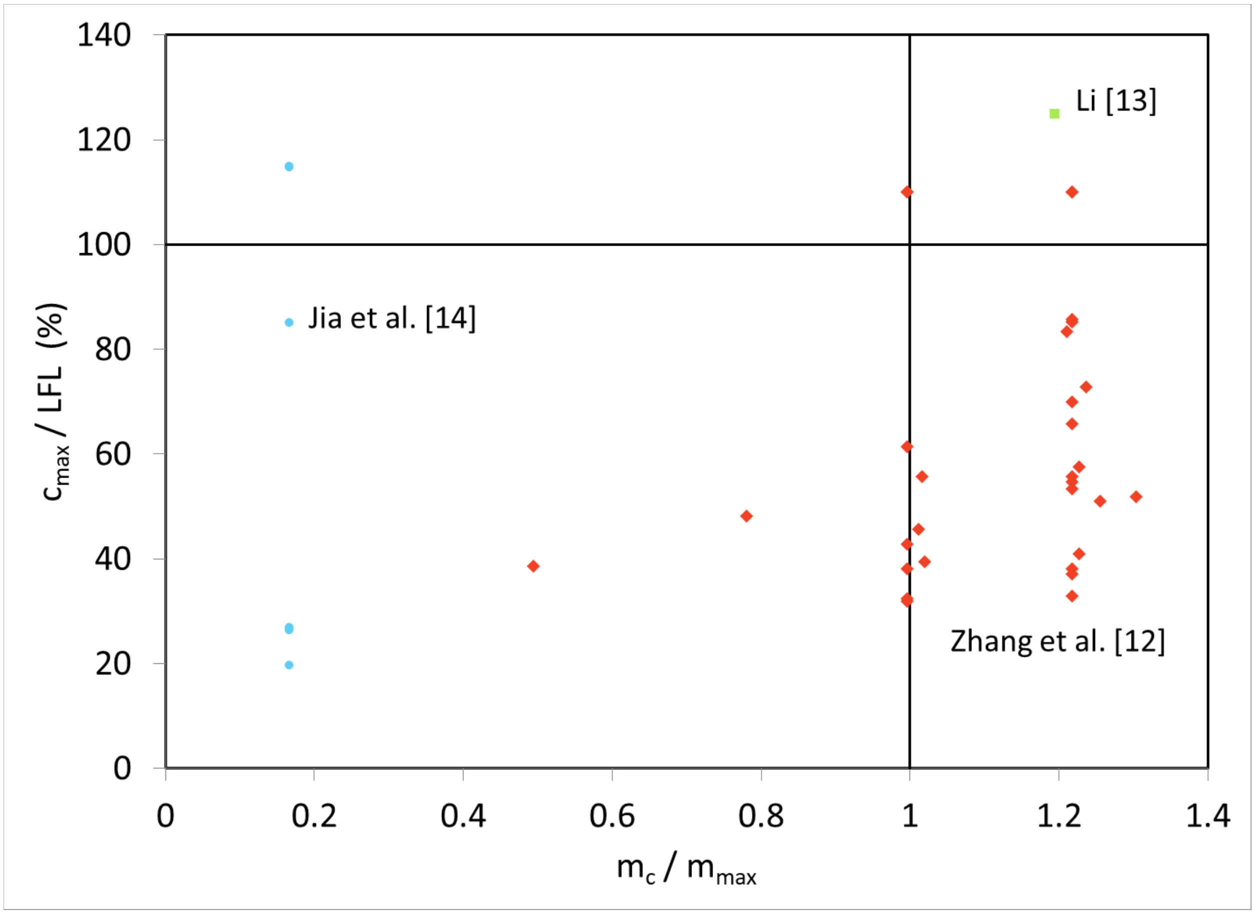


Figure E.1. Pictorial summary of a sample of flammable refrigerant dispersion studies

The main conclusion from the analysis and review of recent experimental and numerical studies was that the results of such studies should directly connect to the corresponding maximum charge as calculated by the pertinent standard, to determine the practical impact of the research. As seen in Figure E.1., there are numerous cases where the refrigerant charge is greater than m_{max} while the maximum observed concentration was less than the LFL. There are also cases with very low refrigerant charge but with observed refrigerant concentration in excess of the LFL. The reference sources note that the maximum concentration measurements are quite dependent upon sensor location.

E.3 COMPUTATIONAL FLUID DYNAMICS SIMULATIONS

The core effort in this project involved simulating various refrigerant release scenarios using computational fluid dynamics (CFD) models. The project team chose to use two commercial software platforms, FLUENT™ and CONVERGE 2.3.17 for these simulations. Results were post-processed using Ensight™ 10.1. The CONVERGE geometry models were built first in SolidWorks™ then exported to CONVERGE STUDIO for CFD simulation setup. To reduce computational requirements, the cases were set up to take advantage of symmetry where possible so that only half the domain needed to be modeled. Three major categories of leak scenarios are described in this report: (1) initial simulations of a leak from wall-mounted air-conditioning (AC) unit into a single room coupled with testing for validation of the

CFD models (section E.3.1), (2) leaks from a package AC unit into a multi-room residential space (section E.3.2), (3) leaks from a small room AC (RAC) unit into a single room (Section E.3.3).

E.3.1 Single Room with Wall-Mounted AC Unit

The room geometry for this scenario is illustrated in figure E.2. Six monitor point locations were created in the model corresponding to the experimental sample locations to allow comparison of measured and predicted refrigerant concentration profiles. An initial set of simulations using this geometry were performed to develop simulation protocols and serve as proof-of-concept. R-32 was used for these initial simulations. The impact of total refrigerant charge (or leak amount), leak flow rate, and leak release height as well as the presence or absence of room obstructions were investigated. A total of 12 cases were constructed to represent a baseline (based on the maximum refrigerant charge allowed per IEC 60335-2-40 and standard leak rates and conditions) and cases exploring release rate, release height, charge quantity, internal obstacle, and ventilation impacts. Table E.2 describes the test cases. The leak release area was specified as a 0.305 × 0.305 m (1 × 1 ft) grate. For simplicity, the leak was modeled as a constant, mass-flow boundary condition across this area for the duration of the leak, which is the time needed for the full charge to leak at the specified rate. Based on a grid-convergence study to optimize accuracy and computational time, a uniform 3.5 cm grid was selected.

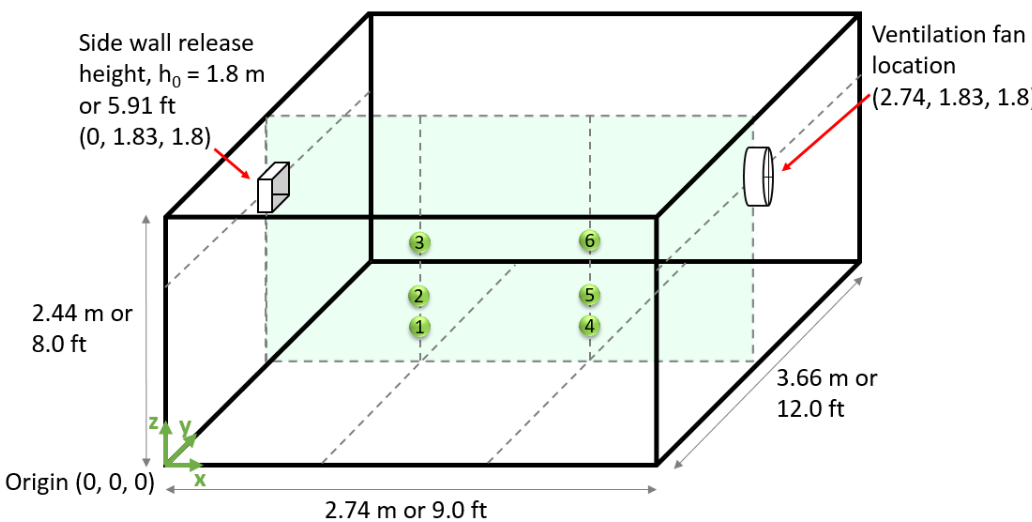


Figure E.2. Geometry model representing the experimental test enclosure used for the single-room, wall-mounted AC simulations. Numbered locations represent monitor points for refrigerant concentration

Table E.2. Simulation parameters for single room with wall-mounted AC

Test #	Refrigerant charge [kg]	Leak rate [g/s]	Resulting leak duration [min]	Leak release area [m^2]	Presence of obstacles	Leak height [m]	Remarks
1	3.257	13.572	4	0.093	None	1.8	Baseline case
2	4.886	20.358	4	0.093	None	1.8	1.5 x higher charge
3	6.515	27.144	4	0.093	None	1.8	2.0 x higher charge
4	3.257	54.289	1	0.093	None	1.8	1 min fast release
5	3.257	5.429	10	0.093	None	1.8	10 min slow release
6	2.172	9.048	4	0.093	None	1.2	Different leak height
7	1.842	7.675	4	0.093	None	0.6	Different leak height
8	3.257	13.572	4	0.093	None	1.8	Liquid leak
9	3.257	13.572	4	0.093	Boxes	1.8	10% occupied
10	3.257	13.572	4	0.093	Boxes	1.8	25% occupied
11	6.515	27.144	4	0.093	None	1.8	Constant exhaust vent fan
12	6.515	27.144	4	0.093	None	1.8	Small mixing fan at release point (180 CFM) + exhaust fan

The simulation results showed significant level of stratification of R-32 concentration. The assumption of uniform distribution of the flow across a large leak area (0.093 m^2) resulted in low-momentum flow of refrigerant entering the room and immediately cascading down the wall under the influence of gravity for all leak rates simulated.

Maximum concentration for Baseline, Case 1, was ~13%, very near the R-32 LFL concentration of 14.4% per ANSI/ASHRAE 34. Doubling the AC unit charge had a significant impact, raising the maximum concentration to more than 23%, exceeding the LFL level. Adding ventilation showed little impact on R-32 concentration near the floor. Figure E.3 illustrates total fraction of the room volume with a flammable concentration of R-32 (concentration between LFL and UFL) vs. time for several of the Cases. For the Baseline Case 1, about 2% of the room volume held a flammable concentration for about 40 s. Case 5 (slow leak) showed no flammable volume. Doubling the charge showed about 50% maximum flammable volume with or without ventilation (Cases 3, 11, and 12). With a fast leak, Case 4, there was ~20% flammable volume. Lowering the release height from 1.5 m to 0.9 m showed also a maximum flammable volume of ~20% but it dissipated more quickly (lower total charge release).

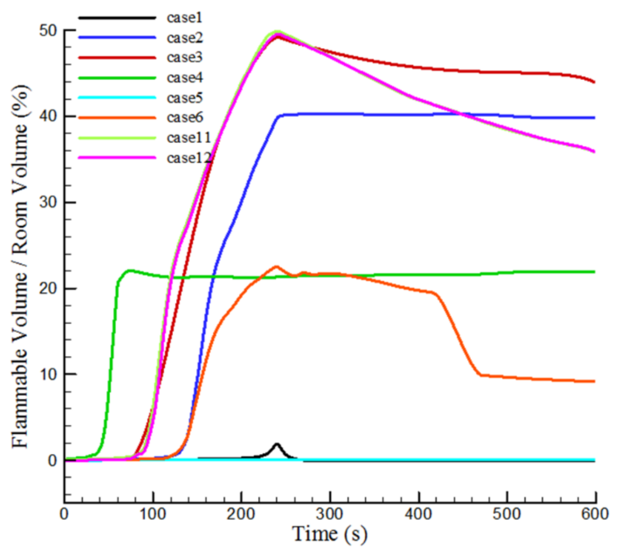


Figure E.3. Flammable charge volume vs. time for Cases 1-6, 11, and 12a (FLUENT results)

To calibrate the proposed CFD models, tests were performed for each case listed in Table E.2 to study the release of flammable refrigerants into a single room for different scenarios and operating conditions. A total of 21 tests were conducted and data were successfully obtained on the diffusion and mixing of refrigerant R-32 when released into a test enclosure having the dimensions illustrated in Figure E.2.

Measured refrigerant concentration gradients in the test room showed that less charge stratification was observed than that predicted by the CFD models in the initial simulations (compare Figures 5 and 20, section 4). As mentioned above, for the initial CFD simulations the leak was applied as a uniform mass-flow boundary condition across the return air grill in the initial simulations resulting in a low-momentum cascade of refrigerant exiting the grill and flowing to the floor producing the high concentration gradients. However, visual observations of the leak release during the calibration testing indicated that the refrigerant entered the test room as a relatively high momentum plume. Therefore, several approaches were tested in CONVERGE to develop a more accurate representation of the observed leak release pattern. By simply varying the area through which the leaked refrigerant enters the room using a square grid ranging in size from 0.305 m to 0.001 m equivalent diameter. It was determined that a release grid of ~25 mm (1 inch) equivalent diameter produced the best match to the observed room concentration measurements, providing a much better match for the cases listed in Table E.2 than the low momentum waterfall release pattern used initially.

E.3.2 Multi-Room Residence with Package AC Unit

This scenario involved simulations of refrigerant releases from a 10.55 kW (3-ton) package AC unit (16 SEER, 3.175 kg (7 lb) charge) connected to duct system serving a 167.23 m^2 (1800 ft^2) 4-room residence. A total of nine cases were simulated, seven with R-32 and two with R-452B. Both floor and ceiling ducts were simulated. Two leak durations were simulated: a slow leak (4-min duration) and a catastrophic) leak representing a rupture of a 6.35 mm (¼”) internal diameter pipe downstream of the evaporator coil. For this case, the leak flow rate was computed to be 0.1786 kg/s (0.393 lb/s). Table E.3 lists the case study parameters.

Table E.3. Simulation parameters for 4-room residential space with package AC unit

Test #	Refrigerant	Remarks[a,b]	Leak duration [s]
1	R-32	All rooms open Floor supply registers	240
2	R-32	All rooms open Ceiling supply registers	240
3	R-32	All rooms open Floor supply registers	17.8
4	R-452B	All rooms open Floor supply registers	240
5	R-32	All rooms closed Floor supply registers	240
6	R-452B	All rooms closed Floor supply registers	240
7	R-32	All rooms closed Floor supply registers	17.8
8	R-32	All rooms closed Floor supply registers Supply air fan on	17.8
9	R-32	Two rooms open & two closed Floor supply registers	17.8

[a]AC unit indoor fan assumed off for all cases except Case 8
[b]No duct leakage assumed for duct simulations

To further improve the computational time, simulation of the refrigerant flow through the duct was conducted separately from that of the refrigerant dispersion throughout the larger space. This approach ensured adequate length scale for both simulation domains without compromising speed or accuracy. The flow leaving the outlets was used as the inlet flow condition for the room space simulations. Note that by doing so we essentially forced the duct simulation solution onto the room simulation. It was implicitly assumed that room air turbulence levels had no significant impact on the air/refrigerant mixture leaving the duct outlets.

For floor duct with standard 4-min leak and unit fan off (cases 1 and 5), essentially no refrigerant was shown to enter the rooms within the 10-min simulation time span. The refrigerant remained in the ducts resulting in a large flammable volume relative to the total duct volume. This combination of high flammable volume within the confines of the ductwork represents a significant fire risk if an ignition point is introduced (e.g., sparking when the system fan turns on). Note that this represents a worst case since no leakage from the ducts to surrounding ambient was assumed for these simulations. In a real case it can be expected that the refrigerant remaining in the duct will eventually escape to the crawlspace or attic and disperse to the outdoors. Still, for a fairly tight, low-leakage duct system, these results indicate a significant likelihood that a flammable volume could persist inside the ductwork for an extended time.

For the room air flow simulations, underfloor ducts with fast leak and AC unit fan off using R-32 showed that the refrigerant volume fraction inside the room was extremely small; the maximum concentration was <0.01% in the space directly above the air grill. With the AC fan on and fast leak time, and AC indoor fan on, the maximum R-32 concentration within the space was ~5.3% (37% of LFL) at points just above the supply registers closest to the AC unit. After the leak end, the fan quickly dispersed the refrigerant throughout the room and refrigerant concentrations ranged from 0.5 to 1.0% at the monitored locations.

In the case of the ceiling duct, case 2, gravity enhanced the flow of the refrigerant. Maximum predicted concentration of the refrigerant inside the duct was ~14% in the vicinity of the leak release point, just below the R-32 LFL concentration.

Results for the Case 2 room simulation showed that during the leak event (first 240 s), the refrigerant was entering the rooms; while afterwards, the refrigerant mass flow rate through the diffusers reversed direction almost immediately. Just before the leak ended, the R-32 concentration maximum in the rooms was ~3.3% or about 23% of the R-32 LFL concentration. At 241 s, room air began to flow into the supply registers while R-32/air mixture flowed into the hallway through the return grille. At 244s, the R-32 concentration near the return grille reached a maximum of ~2.9% (~20% of LFL concentration). At the 10-min point all the refrigerant was evenly dispersed throughout the space at ~0.4% concentration.

E.3.3 Single Room with Small RAC

This CFD simulation scenario focused on studying the leak from a small RAC with R-32 charge of 918 g (~3m^3 x R-32 LFL; LFL in kg/m^3) under four cases for different release heights and leak rates (Table E.4, below).

Table E.4. Simulation parameters for single room with small RAC

Case #	Release height [m]	Leak rate [g/min]
1	1.8	100
2	1.8	200
3	1.8	300
4	0.6	100

Simulations were performed to evaluate the volume fraction of R-32 inside the room (same footprint and dimensions as that used for the simulations summarized in section E.3.1). Six monitoring points (two each at 0.3m, 0.9m, and 1.5m elevations) were used for checking the refrigerant concentration. No ventilation fan operation was used in these simulations.

For case 1, the maximum volume fraction was around 4% (~28% of the R-32 LFL concentration of 14.4%) at the 0.3 m monitoring points at the end of the leak time. The volume fraction gradually increased during the leak event at all monitoring points due to the slow leak rate (550.8 seconds to leak the total charge). For cases 2 and 3, the maximum volume fraction was around 9% and 8% (about 63% and 56% of R-32 LFL) respectively at the 1.5 m elevation monitoring point closest to leak location. For both cases, it is observed that the volume fraction tends to gradually increase while the leak is occurring, then begins decreasing. Case 4 presents a leak from a 0.6 m height source. For this case, the maximum R-32 volume concentration was observed at the two 0.3 m monitoring points, reaching a value of ~7.3% (~51% of R-32 LFL) at the leak end point. This value is almost double the volume fraction seen for case 1 for the same leakage rate. The difference is attributed to the release height change which affects the refrigerant dispersion inside the room. In none of the simulated cases did the refrigerant volume fraction at the monitoring points exceed the LFL value of R-32.

To further characterize the flammability risk for the simulated cases, the flammable volume (which is defined as the volume where R-32 volume fraction is between LFL and UFL) was integrated in space and presented in Figure E.4. For a given release height (cases 1, 2, and 3, all at 1.8 m) the flammable volume size is proportional to the leak rate, while the residence time of the flammable volume is inversely proportional to the leak rate. The maximum flammable volume, ~3 liters, is seen for case 4 (slowest leak rate and low release height, 0.6m) while the minimum flammable volume, ~0.9 liters, is seen for case 1 (slowest leak rate and high release height, 1.8m). For case 4, the leaked refrigerant is released at a lower elevation which concentrates the refrigerant dispersion nearer the floor, increasing its volume concentration and accordingly the flammable volume. After the leak stops, the flammable volume dissipates as the refrigerant continues to mix with the room air. The flammable volume for all cases was observed close to the leak source at the wall.

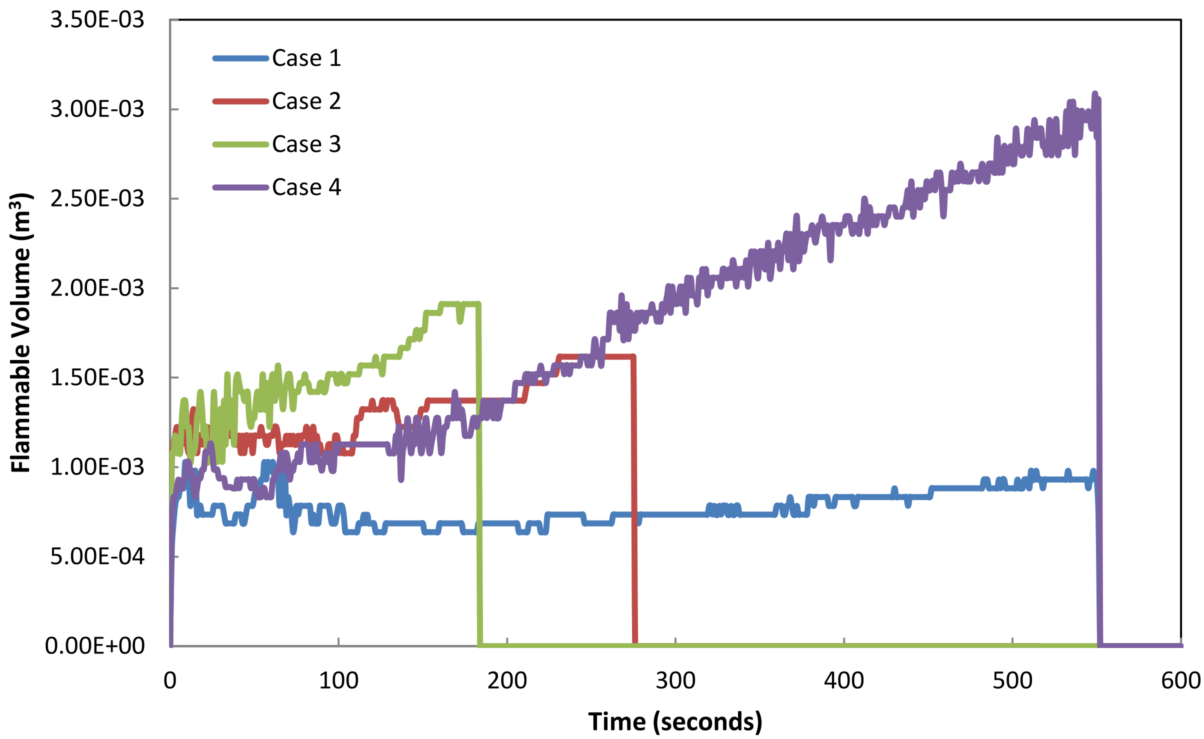


Figure E.4. % volume fraction of R-32 at six monitoring points for case 4

E.3.5 Reduced Order Model (ROM) Simulations and Developments

The final stage of this project involves completing a series of CFD single-room simulations to support formulation of two ROMs (one with unit blower off and a second with the blower on). The goal is to develop a relatively simple approach that industry and safety standards developers can use to estimate safe refrigerant charge limits for a range of refrigerant release parameters. The ROM can be used to develop a correlation based on the parameter given in Table E.6 to estimate refrigerant concentration profiles inside a single room in the case of a leak. Taking this information together with flammability characteristics of a given refrigerant, it should be possible to estimate maximum safe charge limits for that refrigerant. A total of about 600-700 individual CFD simulations will be executed for the ROM development. These simulations are underway, and results will be presented in the second volume of the project report.

Table E.5. Reduced Order Model (ROM) parameters

Parameter #	Parameter	Parameter type	Range
1	Refrigerant type	Continuous	Molecular weight range ~ 44 - 114 g/mol
2	Leak rate	Continuous	3 levels suggested (range 3.75 to 45 kg/min)
3	Room size (volume)	Continuous	Room footprints: 9’ × 12’ base, 12’ × 18’, 18’ × 24’.
4	Leak release height	Continuous	0 m (floor), 0.61 m, 1.22m, 1.83 m, 2.44 m (ceiling)
5	Charge amount	Continuous	0.1 to 15 kg
6	Ventilation	Continuous	~ 0 - 576 cfm
7	Room openings	Continuous	Variable door openings (closed with open floor gap, half-open or door louver, full open)
8	Air circulation	Discrete	Unit blower on or off, 500 cfm

1. INTRODUCTION

Environmental protection goals are becoming progressively more strict to reduce negative environmental impacts of refrigerants. The Montréal Protocol has in the past required phase-outs of chlorofluorocarbons (CFCs, completed in 2010) and hydrochlorofluorocarbons (HCFCs, expected to be complete by 2030 in developed countries). Hydrofluorocarbons (HFCs) like R-410A and R-134a have been used as alternatives to HCFCs for many HVAC&R applications but have relatively high global warming potentials (GWP). In October 2016, the Kigali Amendment to the Montréal Protocol was adopted to phase-down the use of HFCs. For developed countries the Kigali Amendment requires HFC consumption to be reduced to 15% of the average consumption for 2011-2013 by 2036 [1]. Proposed lower GWP alternatives to replace high-GWP HFCs include low-GWP HFCs, hydrofluoroolefins (HFO), hydrochlorofluoroolefins (HCFO), hydrocarbons (HC), ammonia (R-717), CO_2 (R-744), or blends containing low-GWP HFCs, HFOs, and/or HCs. Most of the lower toxicity (class A) low-GWP alternatives are flammable to some degree according to ANSI/ASHRAE 34 [2] and ISO 817 [3], which designate toxicity and flammability of refrigerants as follows:

Table 1. Safety classification of refrigerants as outlined in ISO 817 and ANSI/ASHRAE 34

	Safety group	
Higher flammability	A3	B3
Lower flammability	A2	B2
	A2L*	B2L*
No flame propagation	A1	B1
	Lower toxicity	Higher toxicity

*A2L and B2L are lower flammability refrigerants with a maximum burning velocity of ≤ 10 cm s^{-1}

Refrigerant flammability introduces new challenges to the usage of low global warming potential (Low GWP) refrigerants in real life applications. Those challenges are centered around the deflagration risk associated with their use and its implications on personal safety. Standards have been developed to systematically set maximum allowable flammable refrigerant charges to ensure safety in case of refrigerant leakage. These standards were initially based on limited testing[1] and numerical analyses of refrigerant leakage into confined spaces. Currently published general safety standards include International Standards Organization (ISO) 5149, and its relative counterpart ANSI/ ASHRAE 15

Equipment standards include the International Electrotechnical Commission (IEC) standard suite, IEC 60335-2-24, IEC 60335-2-40 and IEC 60335-2-89. The corresponding CANENA standards are Underwriter's Laboratories (UL) UL 60335-2-24, UL 60335-2-40 and UL 60335-2-89, along with UL 471, UL 563, etc.

These standards were developed based on non-flammable and flammable refrigerant categories. Flammable refrigerants have been included in the IEC and ISO standards for over two decades and have been included more recently in the North American standards. The cognizant bodies for these standards

[1] Clodic, D., and Cai, W., 1996, "Tests and Simulations of Diffusion of Various Hydrocarbons in Rooms from Air-Conditioners and Refrigerators," Proc. IIF - IIR Gustav Lorentzen Conference on Natural Working Fluids - Applications for Natural Refrigerants, Commissions B1, B2, E1 & E2, Aarhus, Denmark.

are engaged in revision/update processes. A main objective of current revision work is to include requirements for the “A2L refrigerant” category in ANSI/ASHRAE 34 and ISO 817 standards.

Most low GWP refrigerant options are either class A2L (lower flammability) or A3 (higher flammability). To enable the deployment of environmentally friendly Low GWP refrigerants, the standards and codes working groups must have reliable, publicly available, science-based data and information to safely use these refrigerants. Information is needed to enable credible safe charge limit estimates for the different flammable refrigerant options for various heating, ventilation, air-conditioning and refrigeration (HVAC&R) applications. Currently, there are gaps in the required information. The goal of this project, Flammable Charge Limits Estimation project, are to 1) prioritize the required information, 3) identify information gaps and 3) fill them in to the extent possible within limits of the project resources.

While expanded use of the low-GWP refrigerants noted above is generally seen as a key to reducing the global environmental impact of HVAC&R equipment and systems, current codes significantly restrict the use of all flammable refrigerants (including lower flammability A2L types) since A2L refrigerants are treated at the same risk level as those in the A2 category in many standards and in some cases, there is no discrimination between any level of flammability. There is, therefore, a need to revise the relevant safety standards and codes to facilitate wider use of low-GWP but flammable refrigerant alternatives; especially A2L refrigerants. However, the bodies responsible for maintaining and updating these standards and codes must have credible, publicly available, science-based knowledge about the safe use of these refrigerants. In particular, information is needed to enable credible estimates of safe charge limits for the different flammable refrigerant options for different HVAC&R applications. Currently, there are significant gaps in this information.

Recognizing this global challenge, the Alliance for Responsible Atmospheric Policy, the Air-Conditioning Heating and Refrigeration Institute (AHRI), ASHRAE, the U.S. Department of Energy (DOE), and the State of California began coordination to develop an effective and efficient program to facilitate development of this information. In 2016, these groups agreed to commit $5.8 million to cover the highest priority research needs: AHRI– ($1 million), ASHRAE ($1.3 million), DOE ($3.0 million), and the State of California ($0.5 million). In 2016, Oak Ridge National Laboratory (ORNL) began a project under this collaboration to investigate a systematic approach to setting safe charge size limits for various types of equipment employing flammable refrigerants.

The primary objective of the project as laid out in the original work scope is to examine the currently imposed charge limits for flammable refrigerant (A2L, A2, and A3) and identify reasonable adjustments to these limits as appropriate. Four tasks were established to work toward accomplishing this goal.

- Gather HVAC&R industry stakeholder input: an initial workshop was organized and held in October 2016 at ASHRAE HQ in Atlanta. In addition, the Air Conditioning, Heating, and Refrigeration Technology Institute (AHRTI) organized a project monitoring subcommittee (PMS) for the project. The PMS met regularly with the ORNL team to review progress and recommend adjustments to the project direction as necessary

- Literature review: review relevant International and North American safety standards related to setting charge limits as well as published scientific studies on experimental and analytical evaluation of refrigerant leak scenarios for a range of HVAC&R systems.

- Leak simulations: based on input from the two tasks above, develop an analysis approach to evaluate refrigerant concentration resulting from refrigerant releases over a range of HVAC&R equipment types, conditioned space layout, leak parameters (leak rates, amounts, release locations, etc.) and different mitigation scenarios. Computational fluid dynamics (CFD) analytical tools were chosen to conduct the analyses.

- Assessment of CFD results and development of reduced order models: critically evaluate CFD results to generate ROM(s) to enable estimation of maximum charge limits for flammable refrigerants in different applications without resort to full CFD analyses.

This report and a follow-up companion report describe the scope, tasks, and relevant results of the project. Section 2 describes results of an initial workshop held to solicit critical input from stakeholders in industry and other organizations to help guide the project and achieve results most useful to the HVAC&R safety standards developers. Section 3 summarizes key results and observations of a review of current and prior literature, patents, etc., highlighting important areas of research which may require additional examination. In sections 4.1 and 4.2, a description of the initial computational fluid dynamics (CFD) studies is provided along with companion calibration and validation results. The calibration work was added to the project plan based on input received at the workshop and from the AHRTI PMS. Section 4.3 provides a discussion of key results from CFD simulations of a representative 4-room single-family house and duct system. Section 4.4 provides a discussion of key results from CFD simulations of a single room with small room air conditions (RAC). Finally, the planned approach for development of the ROM is discussed in Section 4.5. The follow-up report will describe results of CFD simulations conducted for the ROM development as well as the ROMs together with examples of their use for estimation of charge limits.

2. WORKSHOP

ORNL held a workshop on October 24th, 2016 to solicit critical input from stakeholders in industry and other organizations to help guide the project and achieve results most useful to the US HVAC&R and Appliances community. ASHRAE hosted the workshop at its Atlanta Headquarters Offices. Forty invited stakeholders participated joining seven ORNL and DOE staff. The stakeholders included experts from HVAC&R industry OEMs, Appliance industry OEMs, refrigerant manufacturers, standards/codes development organizations, industry and professional organizations, and representatives from DOE and EPA. A list of the attendees is included in Appendix A.

The workshop objective was two-fold: 1) engage the stakeholders in discussions to elicit input regarding gaps in R&D related to safe application of flammable refrigerants, safety standard information/updates needed, critical factors to include in the computational fluid dynamics (CFD) analyses phases of the project, and primary practical issue to consider in the analyses; and 2) identify a few primary case studies or scenarios to be pursued under the project.

2.1 WORKSHOP PROCESS

The workshop program began with an initial presentation that included a discussion of the current and planned revisions of treatment of flammable refrigerants in relevant safety standards particularly Annex GG of the International Electrotechnical Commission standard IEC 60335-2-40 [4], discussion of a literature review of previous work related to flammable refrigerant charge size evaluation and current R&D efforts, and the intended analysis approach. Four breakout sessions followed for detailed discussion of relevant topics. The first breakout session focused on the R&D gaps in the field of flammable refrigerant application. The discussion was centered around the scientific basis and the assumptions upon which the flammable refrigerant charge limits standards were developed and the deciding criteria for charge limits. The second breakout session focused on the scope of the standards and how comprehensive they are. Discussion was centered around what needs to be included in the standards and how relevant information can be relayed to different parties across the value chain; retailers, contractors, service workers and individual users. The third breakout session focused on the most important factors to consider in the CFD analyses to be conducted. The goal of the discussion was to decide on the assumption and the parameters that are critical to the outcome of CFD analysis results. The fourth breakout session focused on the practical aspects that should be considered in CFD analysis. Factors such as the specific leak scenarios to be modeled and inclusion of mitigation strategy were discussed during this session.

Summaries of the breakout sessions were presented by volunteer spokespersons from among the participants during brief full group sessions after each breakout. Ideas and suggestions generated during the breakouts were assigned priorities via vote by the participants. Each participant received 5 votes "stickers" to distribute among priorities as they saw fit. After the breakout sessions, a final session was held to discuss and prioritize the most relevant case studies to be pursued for further analysis. These case studies were also assigned priorities via vote by the participants. In this case, each participant received only one vote.

2.2 WORKSHOP RESULTS

The breakout sessions generated a total of 71 unique suggested priorities to be considered in the project analyses and/or future efforts. During the final session, 4 unique case study priorities were identified. The following section documents results of each breakout session and the final discussion session. Tables 2-5 give the raw outputs from each breakout session and are followed by discussion of the top voted priority initiatives. Finally, each of the proposed case studies and the votes received are presented. In some cases, these priorities have been addressed in the present project and results included in later sections. Others are recommended for follow-on projects or extension of the current project.

Table 2. Ideas and suggestions from breakout session 1a (What are the relevant R&D gaps?)

Idea/suggestion	Votes
Evaluating the severity of refrigerant combustion event	17
Characterization and probability of leaks	16
Minimum worst-case scenario leak rate for each type of equipment	14
Available ignition energy of common electric components	11
Necessity of validating the CFD results	11
Evaluating the need to account for flame velocity in the charge limit equation	10
Accounting for interior obstructions	9
Evaluating catastrophic refrigerant leak with electric failure	7
Understanding the impact of by-products of refrigerant combustion	5
Characterization of two-phase leakage with liquid on the floor	5
Characterization of space (bedrooms, kitchens, machine rooms, etc.)	4
Evaluating sensors' reliability	3
Developing a testing method to determine releasable charge	1
Definition of safety envelope	1
Investigating available experimental data for CFD validation	0
Characterization of the impact of oil presence	0
Correlating the results to other types of equipment where possible	0

2.2.1 Evaluating the severity of refrigerant combustion event

Currently, the criterion of safe installation is based solely on the maximum predicted concentration of refrigerant in air in case of a leak. The rationale is that as long as the maximum concentration does not exceed the lower flammability limit (LFL), the refrigerant-air mixture will not ignite. However, several other factors affect the combustibility of that mixture as well as the probability and the severity of an ignition event. The mass of refrigerant present within the combustibility limits and how long this mass persists directly affects the probability of an ignition event. Heat release and the rate of heat release in case of an ignition event are indications of the magnitude of the resulting potential damage. In addition to providing a prediction of whether maximum refrigerant concentration will exceed LFL, leakage models should also provide an estimate of how much mass will be available to burn and its presence time. Modeling efforts should also account for deflagration models to characterize the heat release and the rate of heat release that will result from an ignition event. This severity of refrigerant combustion events is being investigated in the ongoing **ASHRAE project 1806-TRP**, expected to be completed by mid-2018

2.2.2 Characterization and probability of leaks

The location, size, and orientation of a refrigerant leak will affect its spatial dispersion pattern. One or more of these variables could be the deciding factor of whether the leak results in an unsafe event or not. Statistical data on the frequency of occurrence of leaks is scarce. Sometimes this data is synthesized from different sources or assumptions need to be made. This data is a critical need for probability risk assessment models. Accurate and reliable laboratory and statistical field data on refrigerant leaks need to be compiled to provide the inputs needed. For the field data, a survey tool is needed to facilitate collection of appropriate data from service contractors and manufacturers. Controlled testing of a range of different equipment types to measure characteristics of leak events (leak flow, total charge lost, leak times, liquid/vapor fraction estimates, oil entrainment in leak, etc.) for operating and non-operation situations could be conducted to provide lab data. Both efforts are outside the scope of the present ORNL project but could be conducted under follow-on efforts. ORNL and AHRTI are collaborating on a new AHRTI project (9012) to conduct a laboratory evaluation of leak events in five different systems. This project began in late 2017.

2.2.3 Minimum worst-case-scenario-leak-rate for each type of equipment

The size of a leak source and pressure and temperature of the refrigerant determine the rate of discharge of the refrigerant from the equipment into its surrounding room/enclosure. Smaller rooms lead to higher refrigerant concentrations from a given size leak event with a room of minimum allowable area being the worst case. Leak sources vary in size from pinholes and cracks (the most common) to larger line or component ruptures. Ruptures are less likely to occur but result in much more severe consequences. Pressure and temperature of the refrigerant charge determine the phase of the leaking refrigerant; liquid, vapor, or two-phase. This affects the rate of discharge of the refrigerant from the leakage source. In addition to the size of the leakage source and the phase of the leaking refrigerant, pressure is also an important factor. Up to the choked flow limit, the higher the pressure is, the higher the discharge rate. Reliable data/information about minimum leak rates due to catastrophic failures of each type of equipment assessed in this project is needed to reliably assess the associated risks. Analyses of room space refrigerant concentration profiles due to equipment leakage events has constituted the bulk of the ORNL effort.

2.2.4 Available ignition energy of different common electric components

Electric components such as relays and switches could be ignition sources when they produce sparks. For example, it is not uncommon for sparks to occur when an appliance is plugged into a wall outlet. Other examples of electric components that may produce sparks include switches, relays, and loose wires. Reliable data on the energy content from spark events that might originate from different electric components is needed for accurate quantification of the associated risk. It is worth noting that in a previous study (report DOE/CE/23810-92 [5]) testing of refrigerant ignition by various electric components was conducted. The goal was to find out whether ignition event occurred. Available energy for ignition was not quantified. Furthermore, a previous ASHRAE research project RP-1580 evaluated a range of risk factors for A2L refrigerants in HVAC&R applications including electric components [6]. Further effort on this topic is beyond the scope and resources of the present project.

2.2.5 Necessity of validating the CFD results

Every risk assessment model relies on CFD simulation of a refrigerant leakage to quantify the presence, the location, and in some studies the presence time of flammable volume. CFD is a powerful tool to characterize the dispersion of refrigerant into a space. However, the outcome of CFD models is directly influenced by the setup of the model. The results of a CFD model depend on variables such as what turbulence model is employed and the specified boundary conditions. CFD models employed in risk assessment models must be validated experimentally to ensure that CFD modeling results are a good representation of reality. Previous AHRI [7, 8], and AHSRAE [6] research projects had shown good agreement between CFD and experimental data. The original work scope for this ORNL project did not include any validation/calibration testing efforts. However, after the workshop the project was re-scoped to include a testing component. Setup and results from the tests and CFD simulation calibration/validation results are discussed in Section 4.

Table 3. Ideas and suggestions from breakout session 1b (Do we have enough information in the safety standard?)

Idea/suggestion	Votes
Impact of certification requirements of technicians	18
Developing training modules and standards for servicing flammable refrigerants equipment	17
Impact of UL, ASHRAE and AHRI standards updates timeline vs building code update timeline	11
Split system exclusion from hydrocarbon use	10
Equipment supply chain	8
Operation and storage in small rooms	7
Sensors coupled with units	6
Educating inspectors and equipment owners	5
Impact of room size on refrigerant charge (mc)	5
Impact of joint quality on severity of leakage – ISO 14903	4
DOT shipping standard for A2L-charged equipment	3
Globally harmonized standards	3
Characterization of systems installations	2
Prevention measures for DIY'ers	2
Review ASHRAE service program	1
Refrigerant charge migration during storage periods (AC vs HP)	1
Validation of m_1 in A_{min} using R-32	1
Fire/emergency response of equipment owners as well as responders	1
Mitigation strategies	1
ORNL participation in standard 15 and 15-2	0

2.2.6 Certification requirements of technicians

Risk of ignition can be 100 – 1000 times greater during equipment servicing than during normal operation. This is due to inclusion of the additional risk factor of probability of human error. Currently, HVAC technician certification is not required by all states. Only EPA certification is required. With the introduction of the risk associated with flammable refrigerants, certification requirements need to be revised. It must be ensured that technicians who work on equipment that employ flammable refrigerants are aware of the associated risks. Effort should be expended in making sure they have the competencies needed to accomplish their intended work with minimal increase of risk.

2.2.7 Developing training modules and standards for servicing flammable refrigerant equipment

The increased risk of ignition during servicing is the result of the introduction of risk associated with human error. Wrong use of tools, disregarding warning signs and not replacing safeguards are few examples. Servicing flammable refrigerant equipment requires that technicians follow best practices. These practices need to be developed explicitly for flammable refrigerant equipment. Training modules should be developed explicitly for servicing flammable refrigerant equipment that include these best practices and all the Do/Do Not's that apply in the case of flammable refrigerants.

For both 2.2.6 and 2.2.7 above, we suggest that North American Technician Excellence (NATE) and Air Conditioning Contractors of America (ACCA) take the lead in developing the training materials with support from AHRI/AHAM/ASHRAE/EPA/DOE. A related project, **ASHRAE RP1807**, has developed some guidelines for handling of flammable refrigerants during equipment servicing and installation [9]. Additionally, AHAM has published service guidance for residential RACs and refrigerators.

2.2.8 UL, ASHRAE, AHRI standards timeline vs building code timeline

Several standards and codes that are relevant to the use of flammable refrigerants in HVAC equipment are presently under revision to include 2L specific requirements. The most relevant ones are UL 60335-2-24, -40, and -89; IEC 60335-2-24, -40, and -89; ASHRAE 15 and 15.2; and several codes maintained by the International Code Council (ICC; International Mechanical Code, International Building Code, International Residential Code, etc.). The updated IEC 60335-2-40 was published in January 2018 and the next editions of ASHRAE Standards 15 and 15.2 with 2L specific requirements are undergoing public review in 2018. The ICC has a three-year development cycle, the most immediate of which starts in 2018. This means that the revised IEC, ASHRAE, and UL standards may not be adopted in the ICC model codes until 2021 or perhaps 2024 at earliest. This may be problematic for the industry since the phase out schedule of HFC-22 enforces no production or import in 2020.

2.2.9 Split system exclusion from hydrocarbons

Split systems require on-site welding and they have long refrigerant lines. These factors increase the probability of refrigerant leakage. The amount of refrigerant that resides in the outdoor unit versus the amount that resides in the indoor air handler varies depending on operation circumstances, outdoor and indoor temperatures and time of day. This uncertainty affects the accuracy of the risk assessment. Split system-focused analysis should be done to investigate if the risks with split systems are manageable. If not, split systems (or any system involving field installed refrigerant connections) should be excluded from flammable refrigerants use. This assessment is the focus of Case study 1 (see below).

Table 4. Ideas and Suggestions from breakout session 2a (What are the most important factors to consider in the CFD analyses phase of the project?)

Idea/suggestion	Votes
Release locations	12
Boundary conditions	12
Variable vs. constant leak rate	10
Liquid vs. vapor leak	9
Compressibility vs. incompressibility effect	5
Ignition sources	4
Liquid leak affecting temperature	4
Is post-ignition important?	3
Effect of gravity	3
Low velocity vs. high velocity leak	3
Effect of refrigerant density	3
Oil mixed with refrigerant	3
Does air velocity have an effect on ignition	2
CFD performance in the vicinity of leak	1
Establish a concentration criterion	0
Detection location	0
Choked leaks	0

2.2.10 Release Location

Leakage location has a major effect on refrigerant dispersion pattern. Since refrigerants are heavier than air, they eventually settle near the floor. Hence, release height affects the concentration distribution of the refrigerant. In addition to release height, leak orientation (i.e. horizontal, vertical or at an angle) also directly affects the evolution of the distribution of the leaked refrigerant. CFD models should consider different scenarios of release heights and orientation of different equipment types.

2.2.11 Boundary Conditions

Boundary conditions are important in determining the evolution of leaked refrigerant distribution. Walls and furniture are examples of boundaries that redirect the flow. Air velocity (e.g. from mechanical ventilation or natural convection) and ambient temperature are other examples of boundary conditions that affect the dispersion pattern of the leaked refrigerant. Boundary conditions should be accurately considered in the CFD simulations of refrigerant leakage scenarios.

2.2.12 Variable or constant leak rate

In real life scenarios, the discharge rate of leaked refrigerant decays with time as pressure inside the system depletes. The size of the leakage source, pressure and temperature of the refrigerant in the system and the amount of charge affect the decay. CFD simulation of refrigerant leakage scenarios should consider these factors in order to obtain predictions of leakage dispersion that better predict realistic scenarios.

All the above factors have been considered to some extent for the CFD analyses discussed in later sections of this report (Case study 4, see below).

Table 5. Ideas and Suggestions from breakout session 2b (What are the practical issues that we need to study?)

Idea/suggestion	Votes
Leak rate assumptions	13
Effectiveness of detection and circulation (ducted and ductless)	11
Utility closet	10
VRF (lots of joints)	9
Refrigerant leak in doored display case	8
Ventilation rates; ventilation activation at 25%LFL, 50%LFL etc.?	6
Servicing - release of refrigerant and ignition source (e.g. blowtorch for brazing)	4
Food service	4
Worst case with fan off (also best case for detection)	3
Heating mode/cooling mode (mode of operation)	3
Leak in line sets (in walls)	1
Water-to-water HP	1
Leak in domestic refrigerator	1
Cooling load per ft2	0
Water-to-air HP	0
Heat pump clothes dryer	0
Commercial buildings	0

2.2.13 Leak rate assumption

The rate of discharge of leaking refrigerant depends on the dimension and overall shape of the leakage source, pressure and temperature of the refrigerant in the system, and the mass of refrigerant charge. The latter two factors continuously change until leakage stops. Since the rate of leaking refrigerant release directly affects the dispersion of the refrigerant, leak rate assumptions should be representative of realistic leakage scenarios.

2.2.14 Effectiveness of detection and circulation

The location of refrigerant leak detection sensors and leak circulation patterns are sensitive to the leak nature, location and boundary conditions. Determination of optimal leak detection locations is dependent on an accurate estimation of the gas dispersion scenario. The analyses need to provide information for refrigerant sensor locations to best ensure reliable early indication of refrigerant leakage events.

2.2.15 Utility closet

Equipment location inside utility closets is agreed to be the worst-case scenario due to the typically low ventilation rate and confining nature of such closets. It is expected that refrigerant concentration in such a space would exceed LFL rather quickly. Special attention should be paid to the utility closet scenario.

Issues 2.2.13 and 2.2.14 above have been considered for the CFD analyses done under this project (Case study 4, see below). Issue 2.2.15 was unable to be investigated due to resource limitations but could be done under a follow-on project.

2.2.16 Final Case Studies Session

The following case studies were suggested by the workshop attendees,

2.2.16.1 Case 1: Residential split heat pump air handler unit in utility closet (2 Votes)

This would be a parametric study of the effect of leak rate, velocity, location and size of leak hole on the maximum refrigerant concentration inside the closet. The study should also consider different mitigation strategies and identify effective ones. Seasonal effects on the intra unit charge residence (air handler versus outdoor unit) should also be considered. Different leak scenarios to be modeled were suggested: leakage with the presence of a furnace (hot surface), leakage with the presence of water heater with a standing flame, leakage inside versus outside the air handler. This case will only be included in the scope of the current ORNL project if time/resources permit.

2.2.16.2 Case 2: m_1, m_2 and m_3 (5 Votes)

The current relevant standards define three incremental charge limits based on the room volume and the lower flammability limit (LFL) of the refrigerant in question. They then define requirements based on where the actual charge falls in relation to these incremental limits. The premise is that if requirements are followed, the maximum concentration of refrigerant the room will not exceed LFL in case of refrigerant leakage. Models of scenarios that meet the requirements of the relevant standard need to be developed to validate or invalidate the underlying premise of the standard.

2.2.16.3 Case 3: Leak profiles in various applications of RTU, mini split and VRF units (10 Votes)

This would be a CFD campaign to identify the spatial concentration profiles for different leakage scenarios: point source vs. distributed source, high vs. low velocity, high mass vs. low mass, liquid vs. two-phase vs. vapor, rupture of compressor (high electrical discharge), constant vs. variable leak rate, existence of mitigation vs not.

2.2.16.4 Case 4: Room that meets minimum floor area requirements for m_2 (13 Votes)

Reasonable obstructions would be added to the modeled space to represent a more realistic space. Leakage of mass charge equal to m_2 would be modeled at different leak rates and with different refrigerants. Results would be analyzed to investigate if a function could be created that describes the concentration as a function of refrigerant, charge mass and leak rate.

This case will be the priority focus of the current flammable project at ORNL. It received the highest priority from the Workshop participants and would also address elements of Case studies 2 and 3, above.

3. LITERATURE REVIEW

As indicated in the introduction, an important initial step in the project was to summarize key results and observations of a review of current and prior literature, to highlight important areas of research which required additional examination. The literature consisted primarily of probabilistic risk assessments and experimental/numerical studies involving different flammable refrigerant types, leak scenarios and equipment types. Other pertinent work involved studies of flammable refrigerant thermophysical properties, ignition/burning characteristics etc. A draft journal article of the literature survey was prepared for publication, titled: ***Review of flammable refrigerant charge limits and leak studies***. The paper provided an overview of standards for flammable charge limits, put the existing literature into context and provided recommendations for possible future research avenues. A summary of the draft paper is provided in this section with a listing of the literature review bibliography in Appendix B.

3.1 OVERVIEW OF INTERNATIONAL STANDARDS

Since the introduction of flammable refrigerants, several organizations have developed codes and standards to safely use and transport them. Global standards applicable to refrigeration and air-conditioning equipment using hydrocarbons come mainly from two organizations: The International Standardization Organization (ISO) and the International Electrotechnical Commission (IEC).

The standards (along with corresponding refrigerant classification standards from ASHRAE and ISO) provide information about permissible locations for systems employing flammable refrigerants, corresponding maximum quantities of refrigerant, construction requirements for the mechanical systems and external features associated with installation, such as ventilation and detection. The standard which is most relevant to the current work is IEC 60335-2-40 [4] (which is used along with the most recent version of ISO 5149 [10]). The IEC 60335-2-40 is a standard for safety of household and similar electrical appliances and provides particular requirements for electrical heat pumps, air conditioners and dehumidifiers. As is the case in Europe, North American standards pertaining to flammable refrigerants generally involve adoption of corresponding global standards; the US adoption of IEC 60335-2-40 by UL LLC is called UL 60335-2-40 [11].

In addition to many other requirements, IEC 60335-2-40 provides equations for maximum system charge, minimum room area and minimum ventilation. To determine which equations to use for a given scenario, the expected system charge is first compared to the following charge limits, which are a function of the refrigerant LFL:

$$\begin{aligned} m_1 &= (4m^3) \times LFL \\ m_2 &= (26m^3) \times LFL \\ m_3 &= (130m^3) \times LFL \end{aligned} \qquad (1)$$

NOTE: changes to the constants above are under consideration by the cognizant IEC committee.

Based on this, as well as the installation location and type of ventilation, the relevant sub clause in the standard is identified. The maximum refrigerant charge or minimum room area can be determined for a given application, based on the instructions in the sub clause. To understand the rationale behind the above charge limits and equations in IEC 60335-2-40, the research, analysis and inherent assumptions behind them were examined in detail. The conclusions of the examination were as follows:

1. The above charge limits and equations were developed for mostly A3 and A2 refrigerants. However, as charge limits undergo revision to accommodate newer refrigerants (e.g. there are

proposals to increase the factors in Eq. (1) for A2L refrigerants), the efficacy of the standards must be verified.

2. The most conservative conditions were used at the time of development of the standard: low leak velocity, fixed 4 min leak rate, downward leak direction, tight room, no ventilation, no oil presence, no air flow.

3. The above conditions may prove to be overly restrictive for newer A2L refrigerants which have relatively high minimum ignition energy and low burning velocity, especially if sufficient mitigation is present. It is therefore necessary to conduct further parametric studies on the effect of leak duration, location, velocity, direction, presence/absence of ventilation and air flow.

4. The effect of the presence/absence of obstacles on refrigeration dispersion is also not well understood. This is important, since the localized refrigerant concentration may be increased or decreased near the leak in a room with obstacles present.

For these reasons, a need for further research was established to update the equations for existing flammable refrigerant charge limits in the standards.

3.2 LITERATURE SUMMARY

The literature survey in the draft paper provided a listing of recent experimental and numerical studies describing characterizations of flammable refrigerant leaks in HVAC&R applications and highlighted the important areas of research which required additional examination. Probabilistic risk assessment (PRA) studies were introduced, and a listing of recent PRA studies with specific HVAC&R applications was given. Finally, a listing was provided for international guides that were created by several countries to aid in the safe use, handling and storage of flammable refrigerants.

3.2.1 Experimental and numerical studies

The determination of appropriate charge limits depends on, among other things, information on both the spatial and temporal variation of the local flammable refrigerant concentration in the space in question. Many experimental and numerical studies were found in the literature that determined this for both A2L and A3 refrigerant leak scenarios. These are listed in the draft paper by year, refrigerant type, system type/size/configuration, presence/absence of air flow and ventilation, along with important findings. For most studies reviewed, it was determined that aside from flammable refrigerant concentration and dispersion data, there was no apparent connection to the maximum charge limits prescribed by the standards.

To illustrate that disconnect, example experimental studies of flammable refrigerant releases for room air conditioners (RACs) were first selected from the literature [12-14]. The LFL of the refrigerants in these studies was used to determine the m_1, m_2 and m_3 limits (according to Eq. (1)) from IEC 60335-2-40 [4]. Next, information from the studies about the application type, room size, and refrigerant release location were used to determine the maximum refrigerant charge, m_{max}, (according to the relevant equation from IEC 60335-2-40 [4]). The maximum refrigerant concentration measured by sensors at various locations in the space at any time after release, c_{max}, was also found. The data were found for all the cases considered in the studies and were plotted on a single graph, shown in Figure 1. The x-axis of Figure 1 is the quotient of the actual refrigerant charge used in a given case, m_c, and the m_{max} prescribed by the standard for the room size. The y-axis of Figure 1 is the quotient of c_{max} and LFL.

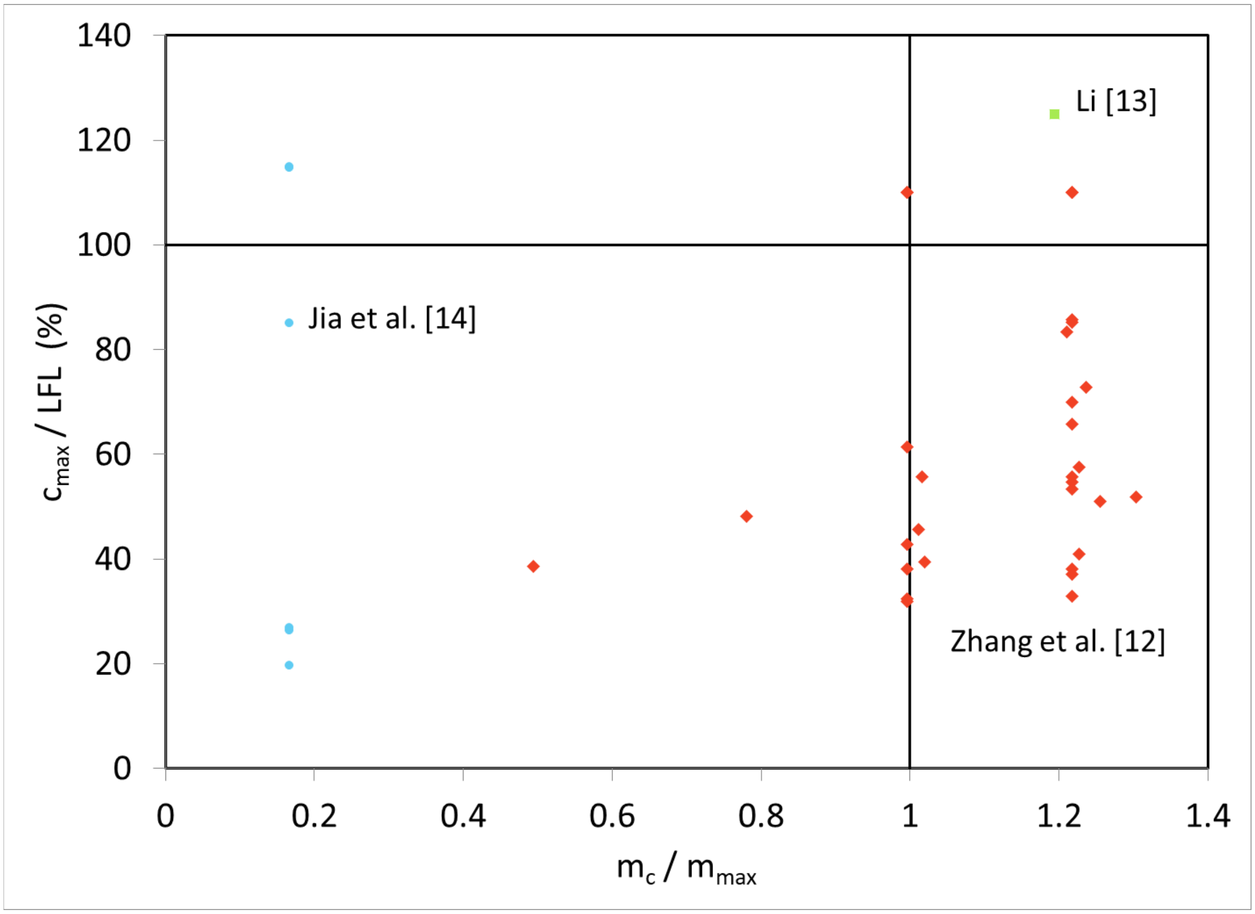


Figure 1. Graph illustrating relationship between flammable refrigerant charge limits (according to standards), actual charge, maximum concentration and LFL for several studies [12-14]

The analysis showed that in many cases, although the maximum refrigerant concentration measured at the given locations at any time after release was below the LFL (i.e. c_{max}/LFL < 100%), the refrigerant charge for the system was greater than the maximum allowable charge per IEC 60335-2-40 (i.e. m_c / m_{max} > 1). At first glance, this indicated that the maximum allowable charge as calculated per the standard was conservative in many of the studies suggesting that charge limits could be increased for at least some applications while keeping the maximum refrigerant concentration below the flammability limit. However, this also strongly depended on the maximum concentration measurement location, since there will always be volumes in the room with concentration between LFL and UFL during a leak (in the immediate vicinity of the leak, for example). As discussed in [13], initial experiments showed that the maximum concentration recorded was below LFL. When the experiments were repeated with the refrigerant concentration sensor at a different location, the maximum concentration exceeded LFL. This highlights the importance of the sensor location.

The main conclusion from the analysis and review of recent experimental and numerical studies was that the results of such studies should directly connect to the corresponding maximum charge as calculated by the pertinent standard, to determine the practical impact of the research. There was also a need for additional research on the effect of changes in the refrigerant concentration sensor location. Although numerical simulations can provide concentration information about the entire field compared to discrete measurements of experiments, their use must be generalized before incorporation into flammable refrigerant charge limit safety standards.

3.2.2 Probabilistic risk assessments of different systems

Probabilistic Risk Assessment (PRA) is a systematic methodology to evaluate risk in an engineered system. In the context of flammable refrigerants, PRA is used to determine severity and probability of a fire or explosion event occurring because of a leak (and subsequent ignition from surrounding sources) of flammable refrigerant from equipment or appliances. Fault Tree Analysis (FTA) is used to quantify likelihood and frequency of such an event occurring.

In the PRA studies found in the literature, complete sets of fault trees were often developed for a particular refrigerant and operating scenario, and the structure of the fault tree was first defined. The input probabilities of lower-level events were determined from various sources. The individual input probabilities were added together, multiplied or combined in more complex ways using logic gates. The most important of these was the probability of refrigerant concentrations reaching the LFL due to a leak, which was found from experimental measurement and CFD simulations of refrigerant concentration mapping. As in the previous section, the PRA studies are listed in the draft paper by year, refrigerant type, system type/size/configuration, presence/absence of air flow and ventilation and important findings.

3.2.3 International guides and resources

In addition to the published journal articles and reports concerning flammable refrigerant leaks and probability risk assessments, various international guides and other resources were also found during the literature review. These have been created in several countries by their respective government entities, industry partners and academic institutions for the safe use and handling of flammable refrigerants. The draft paper provides references for guides created in Japan [15, 16], Germany [17], Great Britain [18] and Australia [19]. The guides provide general information on fundamental studies on flammability limits, refrigerant thermophysical properties, safety studies, physical hazard evaluation and assessments, legal issues with codes and regulations, training of personnel, production and manufacturing facilities, transportation of flammable refrigerants, service and maintenance, emergency planning and marking and labeling.

3.3 RECOMMENDATIONS AND CONCLUSIONS

The literature was sorted according to each HVAC&R equipment type or application, as listed in Table 6. The papers or reports which did not include a specific equipment type or used a point source leak (with the appropriate diameter and location to simulate an equipment leak) are given in the last row. Most of the studies found, ~75%, dealt with air-conditioning (AC) or cooling of human-occupied spaces. Over half (~51%) dealt with relatively smaller single-family home or room ACs or heat pumps. Therefore, much of the emphasis of the review dealt with that application.

Table 6. Number of studies found from literature for each HVAC&R equipment type or application

Application or equipment type	Number of studies found
Split-type air-conditioner or heat pump	19
Packaged or room air-conditioner	8
Commercial rooftop unit (RTU)	2
Variable refrigerant flow (VRF) system	5
Air- or water-cooled chiller	6
Commercial refrigeration	4
Residential refrigeration	3
General point-source leak study	7

The following conclusions were given based on the literature review:

1. Of the studies reviewed in this project, most were for split-type AC (or heat pump) and packaged AC applications. Relatively fewer involved commercial RTUs, VRF systems, chillers and residential/commercial refrigeration. These types of systems have increased probability of flammable refrigerant leakage, risk and consequences due to their large charge amounts and/or larger numbers of field installed tubing joints. Further studies are recommended on these systems, with analysis of worst case scenarios which have the highest probability of leakage or ignition.

2. Important factors which affect the dispersion of flammable refrigerant leaks are not captured in the experimental and numerical studies found. Discrepancies exist between the results of CFD simulations and experimental measurements. For example, ideal conditions used in simulations do not often capture effects such as air currents due to leakage of refrigerant itself and presence of two-phase flow in the refrigerant release. Further studies are recommended to revise simple models (which can be validated by experimental results and observation) that account for phase-change, flashing and other dynamics.

3. Current methods of experimentally measuring spatial refrigerant concentration at discrete points do not account for local air circulation and currents near the sampling location, which impact the concentration, resulting in large uncertainty. Recommendations to address these issues include (1) using advanced measurement techniques with higher precision for the entire flow field, such as Particle Image Velocimetry (2) use of a tracer gas to give detailed concentration at many points.

4. In CFD simulations, it is recommended that the concentration near a leak be averaged over a small volume with time (e.g. spherical volume), instead of a single discrete point. This can allow for the effects of local air velocity on concentration to be captured.

5. Verification and validation of the flammable refrigerant concentration via experimental measurement and CFD is extremely important, since it is a major component in the calculation of flammable refrigerant charge limits for international standards, which affect all facets of HVAC&R equipment design, installation and use. It is also used as an input in PRAs, and along with ignition, is a major driver for risk in a system. Uncertainty in this quantity can lead to flammable refrigerant charge limits being too restrictive or not restrictive enough.

6. The criterion of safe installation is often based solely on the maximum predicted concentration of refrigerant in air in case of a leak. However, several other factors affect the combustibility of a mixture as well as the probability and the severity of an ignition event, such as the amount of

mass present within the combustibility limits and for how long it persists. Heat release and the rate of heat release in case of an ignition event are indications of the magnitude of the resulting potential damage. Leakage models need not only predict if maximum concentration will exceed LFL but also how much mass will be available to burn and its presence time. Modeling efforts should also consider deflagration to characterize the heat release and the rate of heat release that will result from an ignition event.

7. Risk assessments should consider severity and consequences of ignition on human health and safety, in addition to probability of ignition. Although some studies develop risk maps based on statistical data and other information, many risk assessments only give the probability of ignition.

8. Few studies have been conducted from the perspective of the flammable refrigerant charge limit standards themselves. As a result, even with a wealth of literature on flammable refrigerant leaks, there is no clear consensus on whether the flammable refrigerant charge limits are appropriate or effective for different scenarios. Further research is recommended by starting with existing charge limits as a baseline and working backwards to determine whether they result in flammable refrigerant concentrations, for various scenarios, applications and refrigerant types.

9. A comprehensive US guide for handling flammable refrigerants (as are already available in several countries) from cradle to grave, including training of technicians, transportation and storage is needed.

4. COMPUTATIONAL FLUID DYNAMICS SIMULATIONS

The core effort in this project involved simulation of a range of refrigerant release scenarios using computational fluid dynamics (CFD) models. Two commercial software platforms, FLUENT™ ver. 17.2 [20] and CONVERGE 2.3.17 [21] were used. Results were post-processed using Ensight™ 10.1 [22]. The CONVERGE geometry models were built first in SolidWorks™ [23] then exported to CONVERGE STUDIO for CFD simulation setup. To reduce computational requirements, the cases were set up to take advantage of symmetry where possible so that only half the domain needed to be modeled. Common simulation parameters used for all simulated cases are listed in Table 7. The compressible flow solver was chosen by the team based on high Mach number levels at the leak points and prior experience with CONVERGE in modeling other flow field problems.

Table 7. CFD simulation setup parameters common to all cases

Equation of state	Ideal gas
Solver	Transient
Gas Flow Solver	Compressible
Body Force (m/s^2)	9.81
Turbulence Model	Standard $k - \varepsilon$
Pressure-Velocity Coupling	Pressure implicit with splitting of operators (PISO)
Initial Time Step (Second)	1e-05
Minimum Time Step (Second)	1e-07
Maximum Time Step (Second)	0.5
Total Simulation Time (Second)	600

Three major leak scenarios were modeled in this project: (1) wall-mounted air-conditioning (AC) unit into a single room, (2) package AC unit into a multi-room residential space, (3) small room AC (RAC) unit into a single room. The first scenario was modeled using both FLUENT and CONVERGE with results from an experimental effort used to calibrate the models. Both software tools were found to produce similar results but CONVERGE provided faster throughput of simulation cases due to the availability of multiple license seats allowing parallel jobs. Therefore, CONVERGE was chosen as the platform for all subsequent simulations.

A uniform square grid mesh was used for the flow field domain for each of the three scenarios above. Details of the mesh varied somewhat since the simulated volumes for each case varied considerably.

- Scenario 1: cell size 0.035m grid with approximately 300,000 total cells.
- Scenario 2, duct simulations: cell size 0.025m grid with approximately 95,000-125,000 total cells (different duct geometries were used)
- Scenario 2, room simulations: cell size 0.1m grid with approximately 225,000-445,000 total cells.
- Scenario 3: same as scenario 1

4.1 SETUP AND INITIAL RESULTS FOR SINGLE ROOM WITH WALL-MOUNTED AC UNIT

The initial simulation scenario consists of a wall-mounted AC unit leaking refrigerant into a single room. A complimentary experimental effort (described in Section 4.2) was used to provide calibration data for the simulations to aid in development and proof-of-concept of the modeling effort. The main purposes for this first group of simulations were to establish the simulation parameters (grid size, etc.) and to validate the numerical tool and methodology with the experimental data acquired.

4.1.1 Initial case setup

The room geometry for this scenario was chosen to match the test enclosure used in the calibration experiments. Figure 2 provides important room dimensions along with the x and y location of the leak release point (height was varied) and the location of a ventilation opening on the opposite wall. Six monitor point locations (see Table 8) were created in the model corresponding to the experimental sample locations to allow comparison of measured and predicted refrigerant concentration profiles.

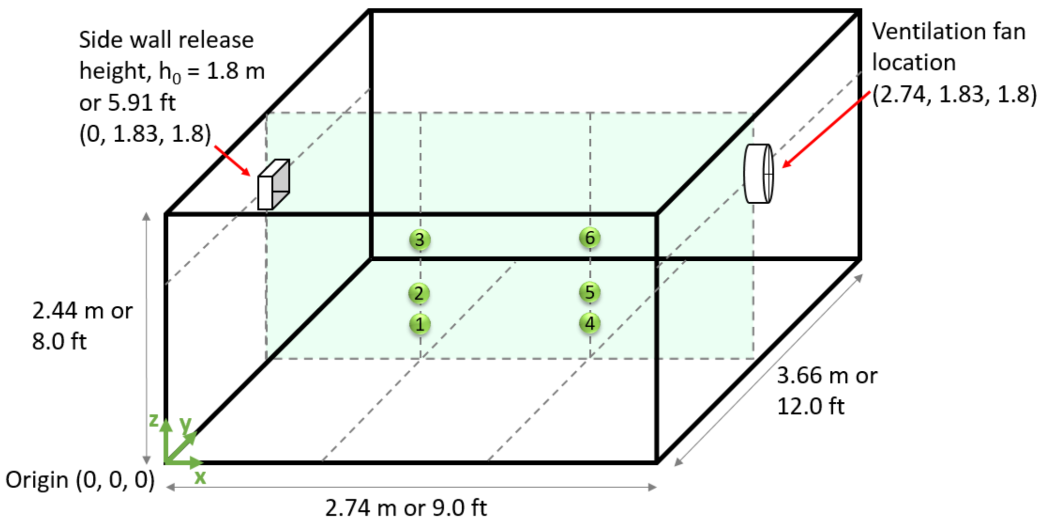


Figure 2. Geometry model representing the experimental test enclosure used for the single-room, wall-mounted AC simulations. Numbered locations represent monitor points for refrigerant concentration and correspond to experimental sample locations (compare to Figure 17).

Table 8. Monitor point locations

Concentration measurement locations	x [m]	y [m]	z [m]
1	1.0	1.83	0.3
2	1.0	1.83	0.9
3	1.0	1.83	1.5
4	2.0	1.83	0.3
5	2.0	1.83	0.9
6	2.0	1.83	1.5

Table 9 gives some properties of the flammable refrigerants considered in the simulation effort along with the maximum and minimum charge limits as prescribed in the current version of IEC 60335-2-40 [4] for the specific room dimensions given in Figure 2.

Table 9. Charge limits for some flammable refrigerants of interest based on room dimensions in Figure 2

Refrigerant	ASHRAE 34-2016 safety group	Lower flammability limit (LFL), % by volume*	LFL, kg/m^3 (at sea level)*	m_1, kg ($3m^3 \times$ LFL)	m_{max}, kg
R-290 (propane)	A3	2.1	0.038	0.114	0.239
R-32	A2L	14.4	0.307	0.921	3.257
R-452B	A2L	12.0	0.360	1.080	3.974
R-1234yf	A2L	6.2	0.300	0.900	3.164
R-1234ze(E)	A2L	6.2	0.300	0.900	3.164

*per ANSI/ASHRAE Standard 34-2016 [2]

The maximum charge limit, m_{max}, in Table 9 is calculated using the following equation from IEC 60335-2-40 [4]

$$m_{max} = 2.5 \times (LFL)^{\left(\frac{5}{4}\right)} \times h_0 \times (A)^{\left(\frac{1}{2}\right)} \tag{2}$$

where A is the room floor area, 10.03 m^2 (108 ft^2), h_0 is the release height, 1.8 m (~6 ft), and m_{max} is in kg.

An initial set of simulations using the single-room geometry were performed to develop simulation protocols and serve as proof-of-concept. R-32 was used for these initial simulations. The impact of total refrigerant charge (or leak amount), leak flow rate, and leak release height as well as the presence or absence of room obstructions were investigated. The leak release area was specified as a 0.305×0.305 m (1×1 ft) grate. For simplicity, the leak was modeled as a constant, mass-flow boundary condition across this area for the duration of the leak, which is then simply the time needed for the full charge to leak at the specified rate. Based on a grid-convergence study to optimize accuracy and computational time, a uniform 3.5 cm grid was selected. Table 10 summarizes the input physical parameters for the simulated cases from this part of the study.

Table 10. Simulation parameters for single room with wall-mounted AC

Test #	Refrigerant charge [kg]	Leak rate [g/s]	Resulting leak duration [min]	Leak release area [m^2]	Presence of obstacles	Leak height [m]	Remarks
1	3.257	13.572	4	0.093	None	1.8	Baseline case
2	4.886	20.358	4	0.093	None	1.8	1.5 x higher charge
3	6.515	27.144	4	0.093	None	1.8	2.0 x higher charge
4	3.257	54.289	1	0.093	None	1.8	1 min fast release
5	3.257	5.429	10	0.093	None	1.8	10 min slow release
6	2.172	9.048	4	0.093	None	1.2	Different leak height
7	1.842	7.675	4	0.093	None	0.6	Different leak height
8	3.257	13.572	4	0.093	None	1.8	Liquid leak
9	3.257	13.572	4	0.093	Boxes	1.8	10% occupied
10	3.257	13.572	4	0.093	Boxes	1.8	25% occupied
11	6.515	27.144	4	0.093	None	1.8	Constant exhaust vent fan
12	6.515	27.144	4	0.093	None	1.8	Small mixing fan at release point (180 CFM) + exhaust fan

Figure 3 shows the half-room simulation domain layout for cases 9 and 10 where 10% and 25% of the room space is occupied, respectively.

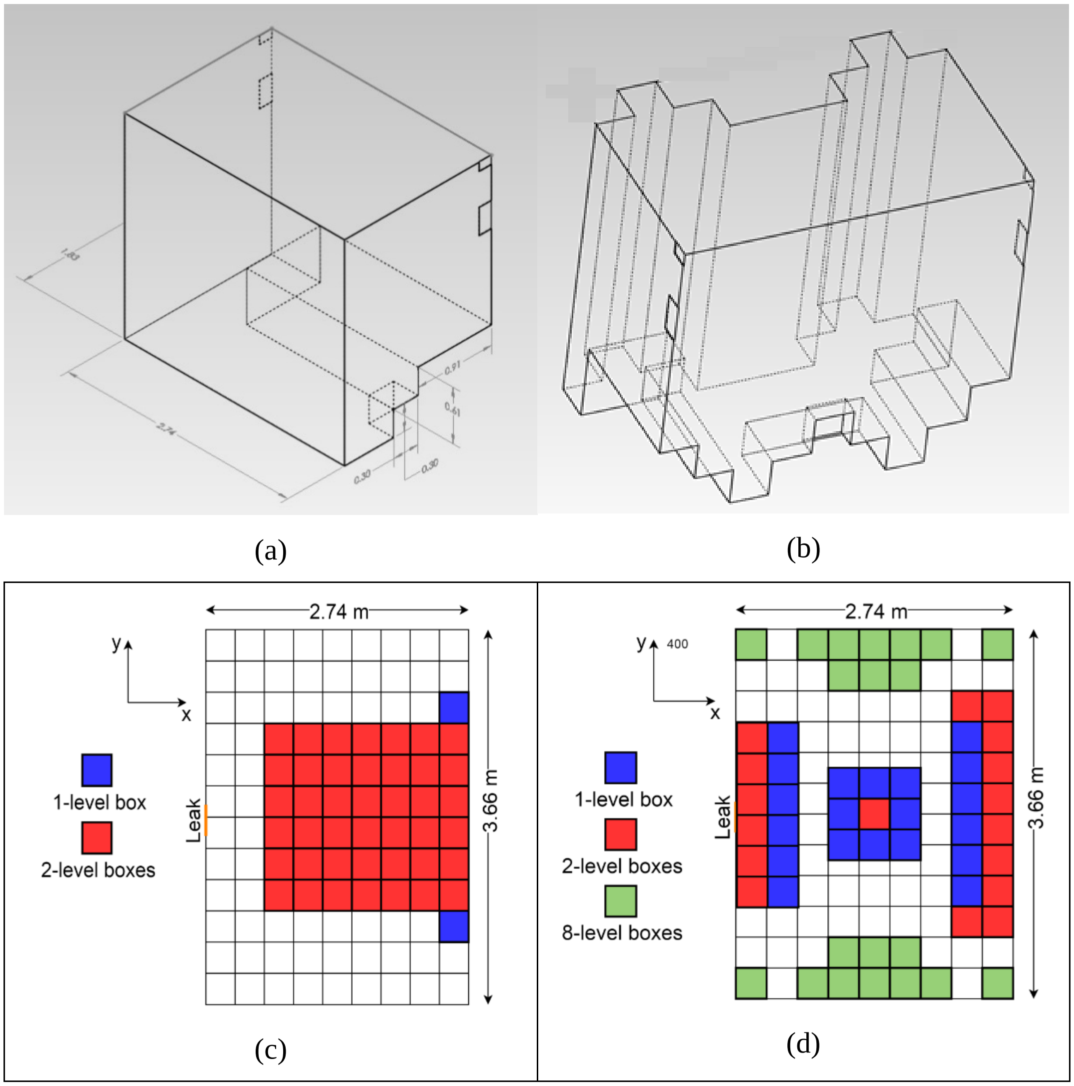


Figure 3. Geometry model of half-room simulation domain for (a.) Case 9 with 10% of room volume occupied and (b.) Case 10 with 25% of room volume occupied. Plan views (c) and (d) show obstacles represented by cubic boxes, 0.305 m (1 ft.) on each side for 10% and 25% obstruction cases, respectively.

4.1.2 Initial case simulation results

Figures 5 - 15 below illustrate R-32 concentration results at the six monitoring point locations (Table 8) for all cases except Case 8 (liquid leak) from Table 10. We have been unable to date to successfully complete a simulation of Case 8. Only the CONVERGE simulations were run for Cases 9 and 10 (with obstacles) with FLUENT simulation results given for the other cases. CONVERGE simulations produced similar results as FLUENT, generally showing lower maximum concentrations (not shown here). Two figures (Figure 14 and Figure 15) are shown for Case 11; one with constant ventilation and a second with ventilation delayed until the R-32 concentration reached 10% at some point in the room. All the results show a significant amount of stratification in the R-32 concentration for all the cases (less so for the slow leak Case 5) with much higher concentrations near the floor. The refrigerant leak was assumed to originate inside the AC unit near the evaporator, wind its way around the coil and other internal components, and finally exit through the unit return air grill. In the simulations, the leak was represented by a constant mass-flow boundary condition applied uniformly across the return air grill. As a result of the uniform distribution of the flow across a large leak area (0.093 m^2), the simulations predict a low-momentum flow of refrigerant entering the room and immediately cascading down the wall under the influence of gravity for all leak rates tested (see Figure 4).

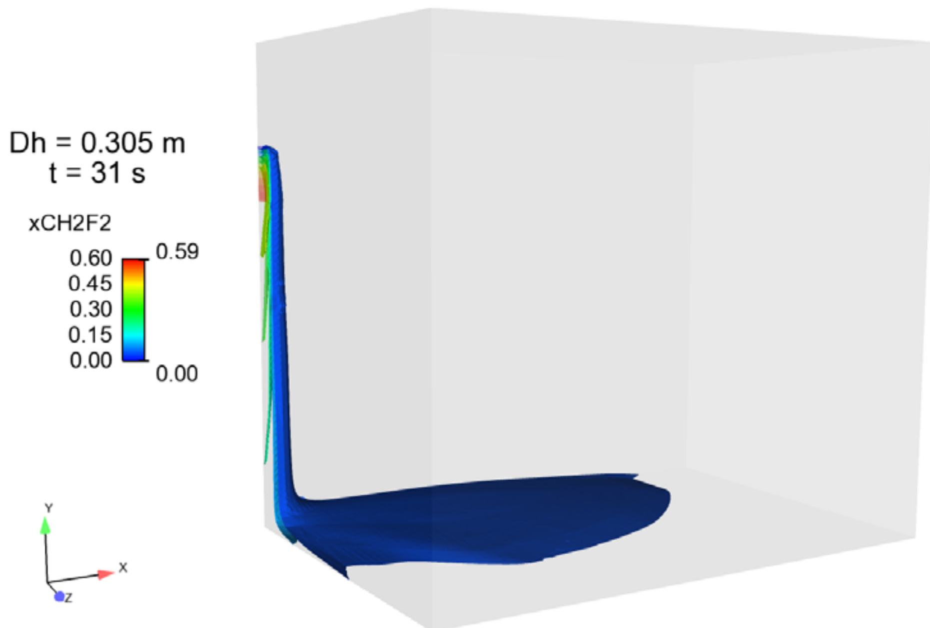


Figure 4. Refrigerant flow entering room from 0.305 m × 0.305 m leak area for initial simulations

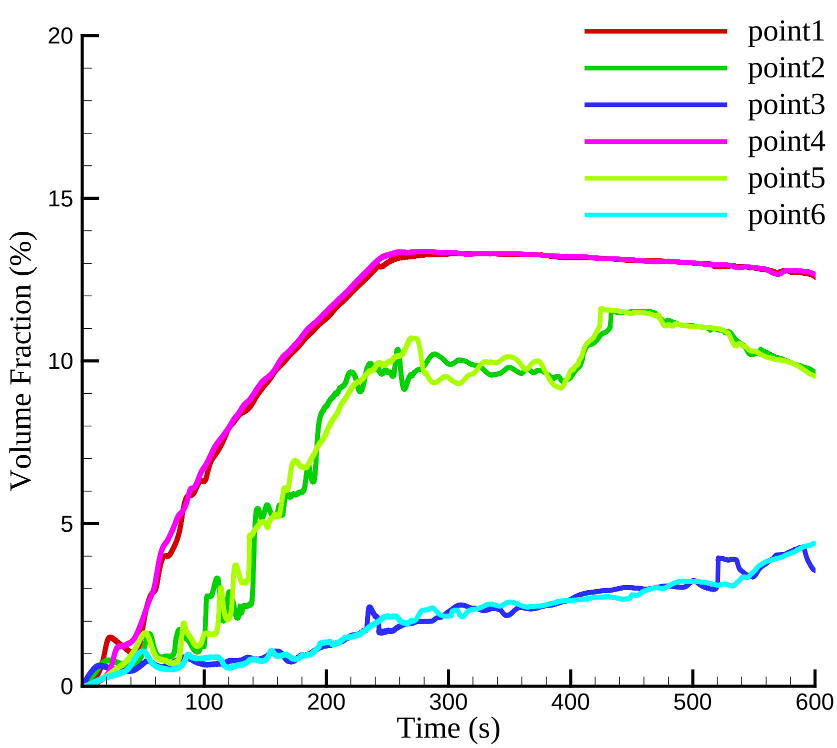


Figure 5. FLUENT Case 1 (Baseline) results for R-32 volume fraction vs. time

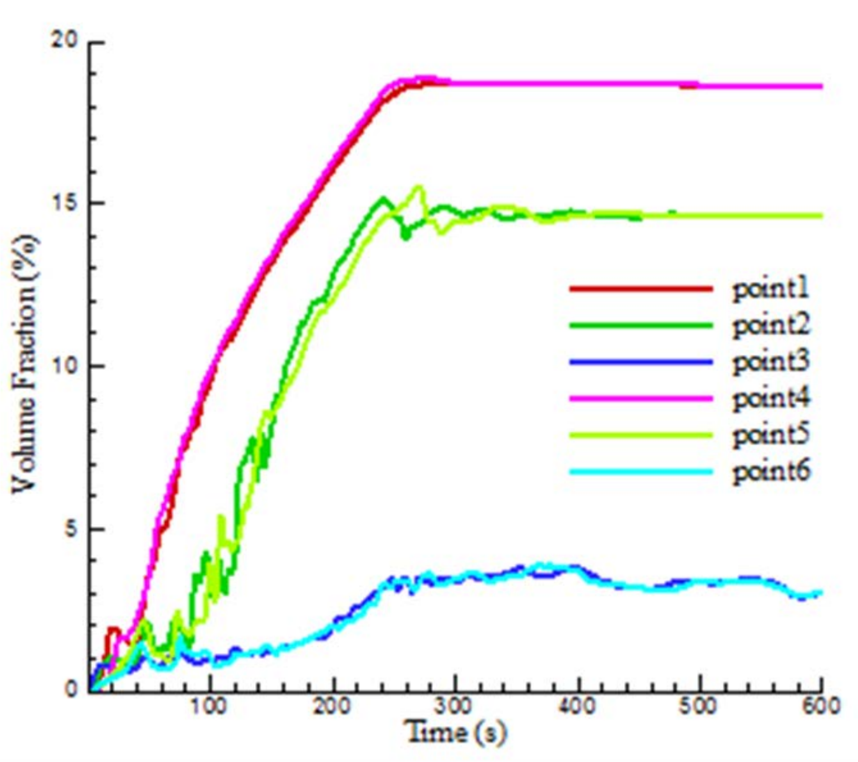


Figure 6. FLUENT Case 2 (1.5 × Baseline charge) results for R-32 volume fraction vs. time

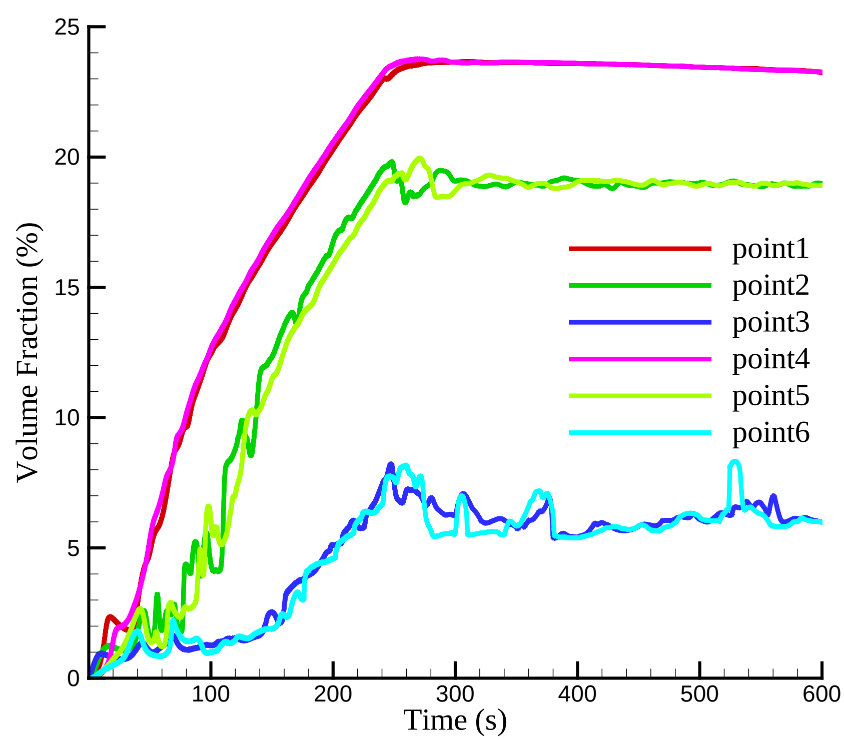


Figure 7. FLUENT Case 3 (2 × Baseline charge) results for R-32 volume fraction vs. time

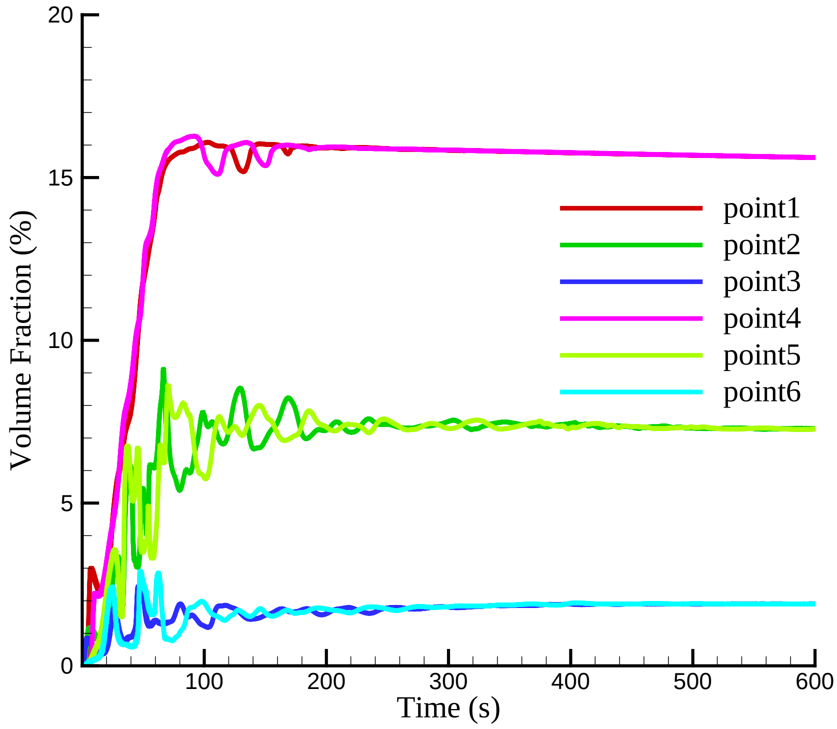


Figure 8. FLUENT Case 4 (fast leak) results for R-32 volume fraction vs. time

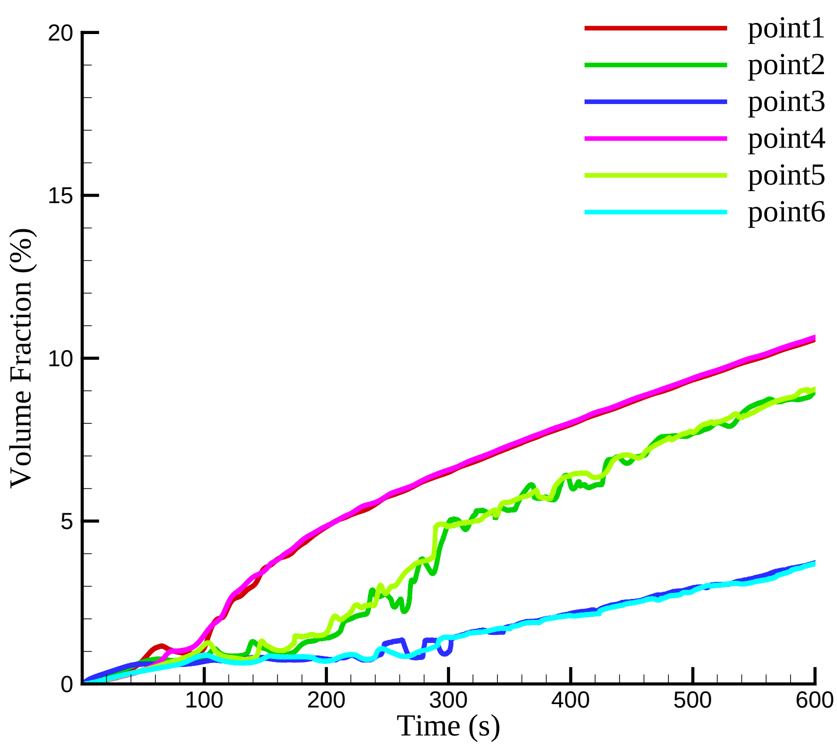


Figure 9. FLUENT Case 5 (slow leak) results for R-32 volume fraction vs. time

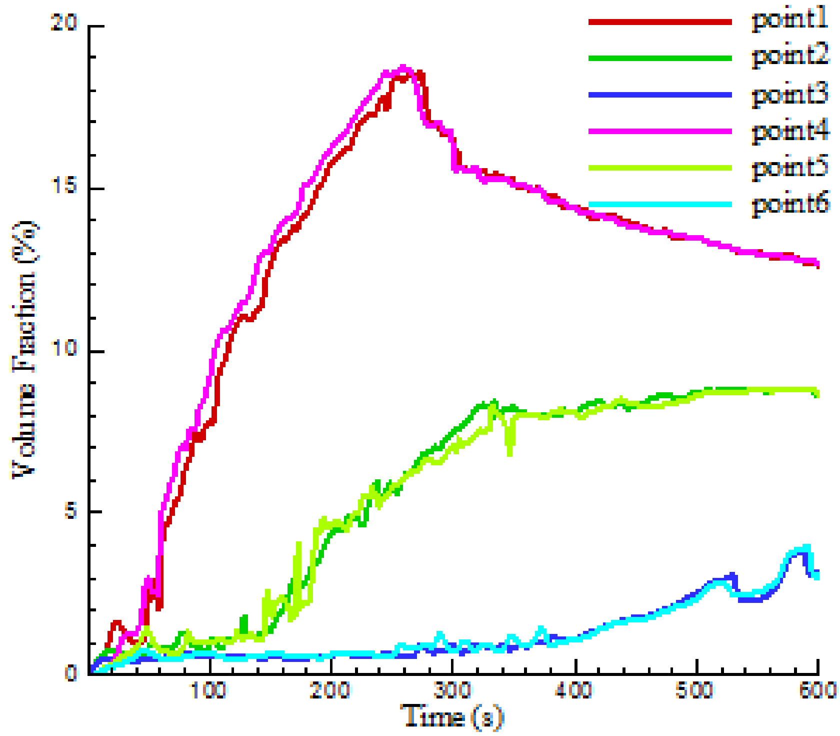


Figure 10. FLUENT Case 6 (0.9 m release height) results for R-32 volume fraction vs. time

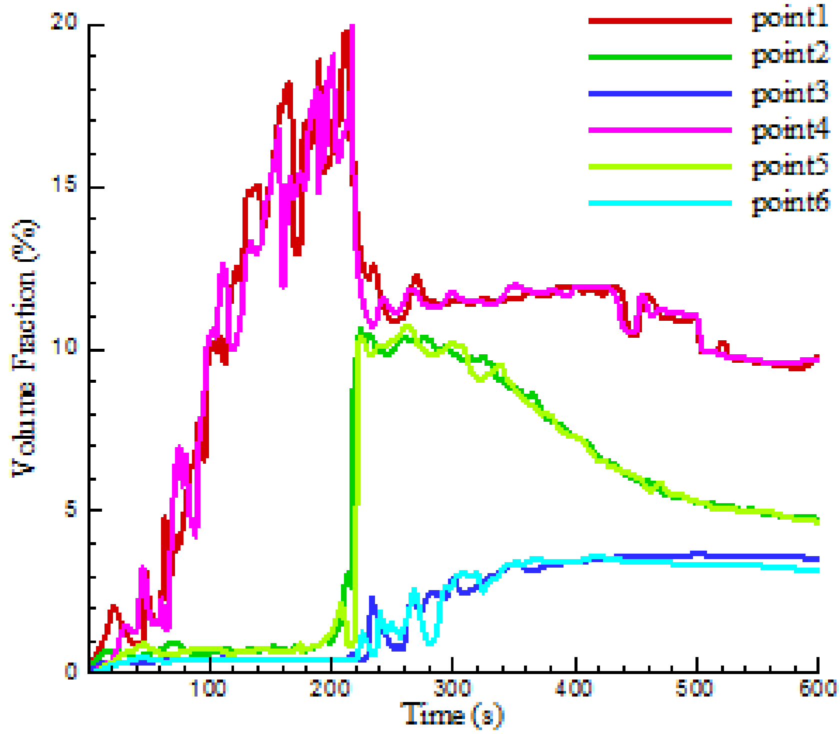


Figure 11. FLUENT Case 7 (0.6 m release height) results for R-32 volume fraction vs. time

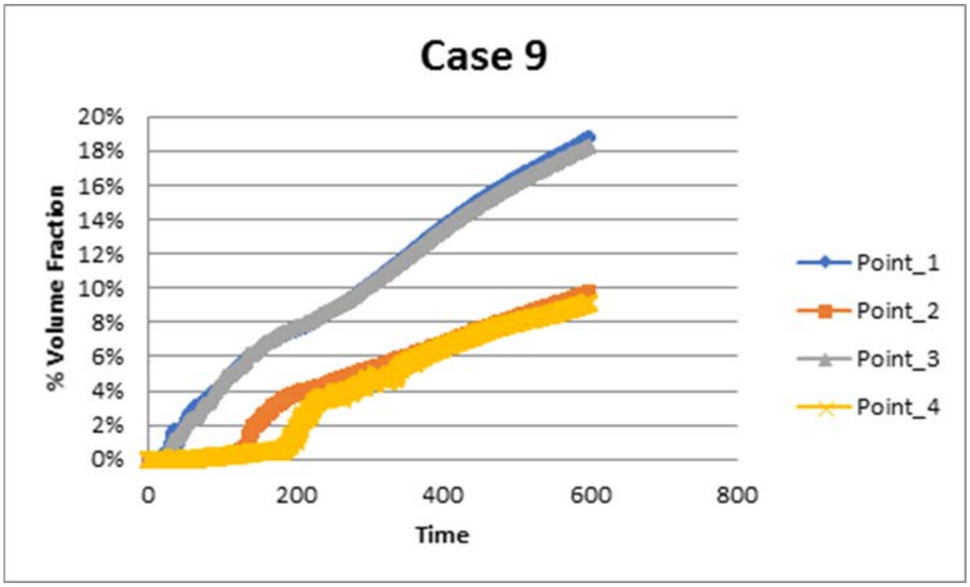


Figure 12. CONVERGE Case 9 (10% obstacles) results for R-32 volume fraction vs. time

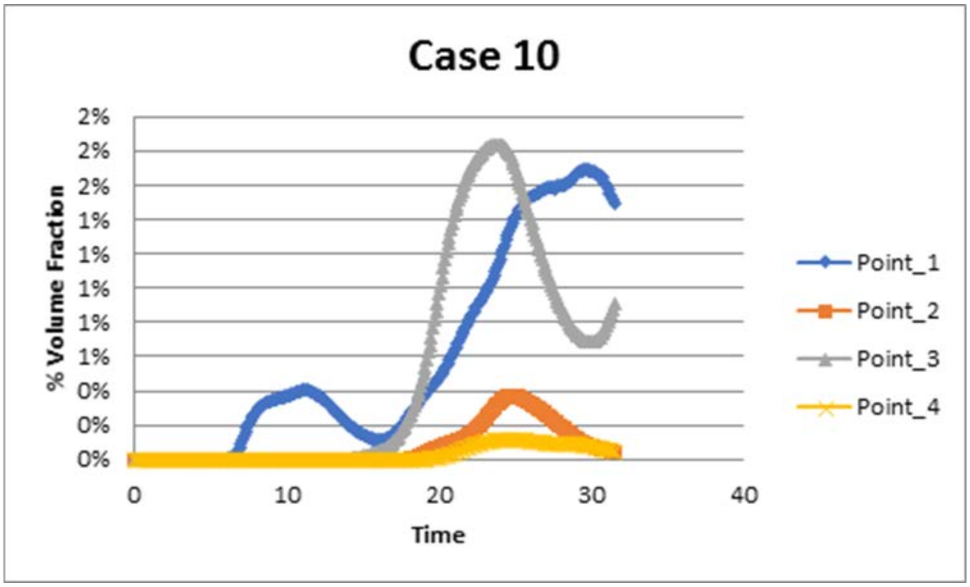


Figure 13. CONVERGE Case 10 (25% obstacles) results for R-32 volume fraction vs. time (only completed first 32s of simulation)

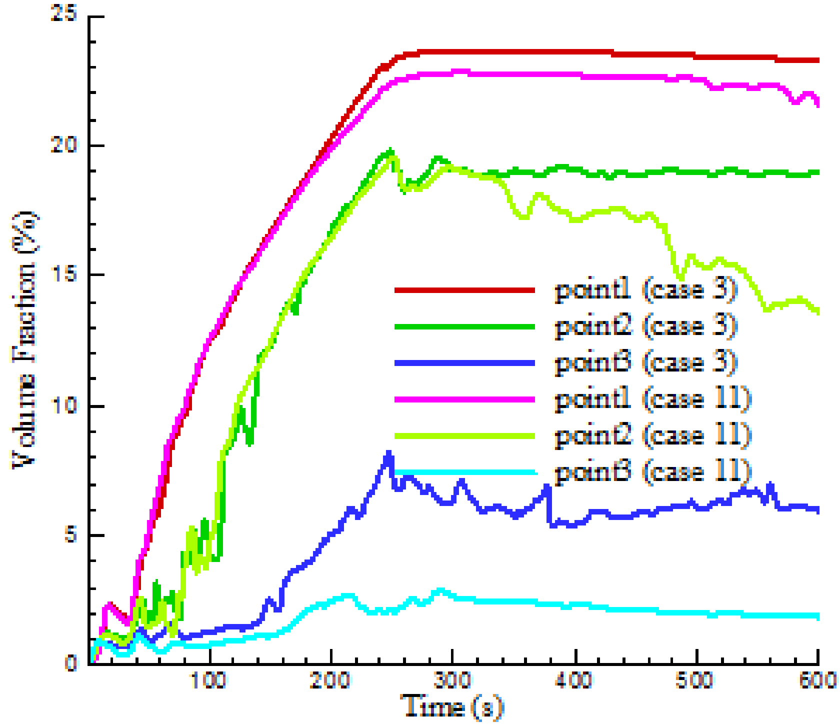


Figure 14. FLUENT Case 11 (2 × Baseline charge with ventilation) results for R-32 volume fraction vs. time

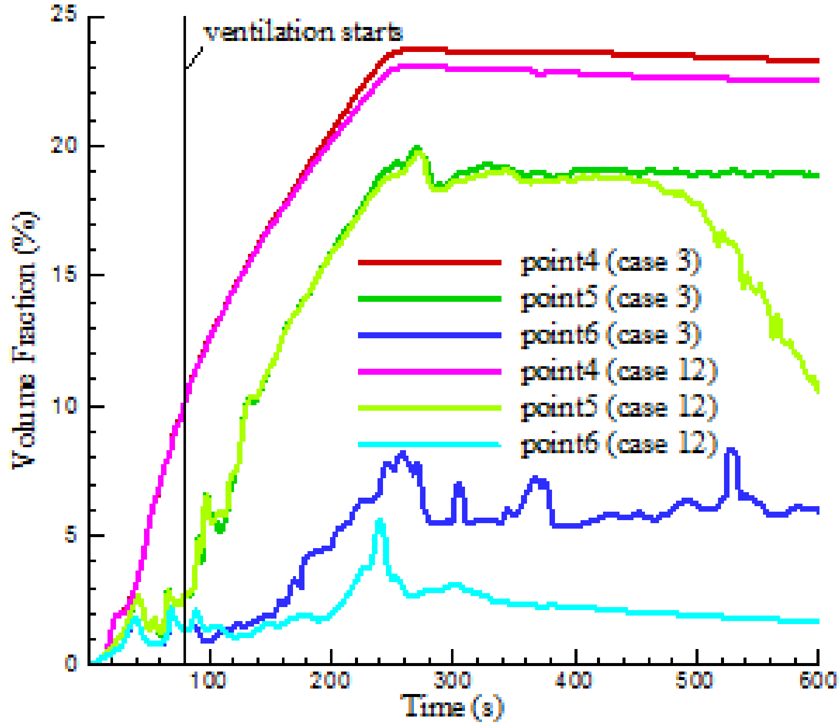


Figure 15. FLUENT Case 11 with delayed ventilation results for R-32 volume fraction vs. time

Maximum concentration for Baseline, Case 1, from the FLUENT simulations was ~13%, very near the R-32 LFL concentration of 14.4% per ANSI/ASHRAE 34 [2]. Increasing the AC unit charge (Figures 6 and 7) significantly increased the maximum concentration (to more than 23% for Case 3). CONVERGE results were qualitatively similar but with somewhat different maximum concentration levels. Adding ventilation showed little impact on R-32 concentration near the floor (Figures 14 and 15). Having the room ventilation fan located at 1.8 m elevation likely contributed to this result. The high extraction location was not effective in reducing concentration near the floor due to the weight of R-32 vs. air. Delayed ventilation (Figure 15) showed almost the same concentration profile as constant ventilation (Figure 14). FLUENT results for lower release heights (Figures 10 and 11) showed higher maximum concentrations near the floor compared to the Baseline (Figure 5), whereas CONVERGE results (not shown) did not show much difference.

Figure 16 illustrates total fraction of the room volume with a flammable concentration of R-32 (concentration between LFL and UFL) vs. time based on FLUENT simulations for several of the Cases. [NOTE: Case 12 in Figure 16 is actually Case 11 with delayed ventilation start.] For the Baseline Case 1, about 2% of the room volume held a flammable concentration for about 40 s. Case 5 (slow leak) showed no flammable volume. Doubling the charge showed about 50% maximum flammable volume with or without ventilation (Cases 3, 11, and 11 with delayed ventilation fan start). With a fast leak (Case 4) there was ~20% flammable volume. Lowering the release height from 1.5 m to 0.9 m (Case 6) also showed a maximum flammable volume of ~20% but it dissipated more quickly (lower total charge release).

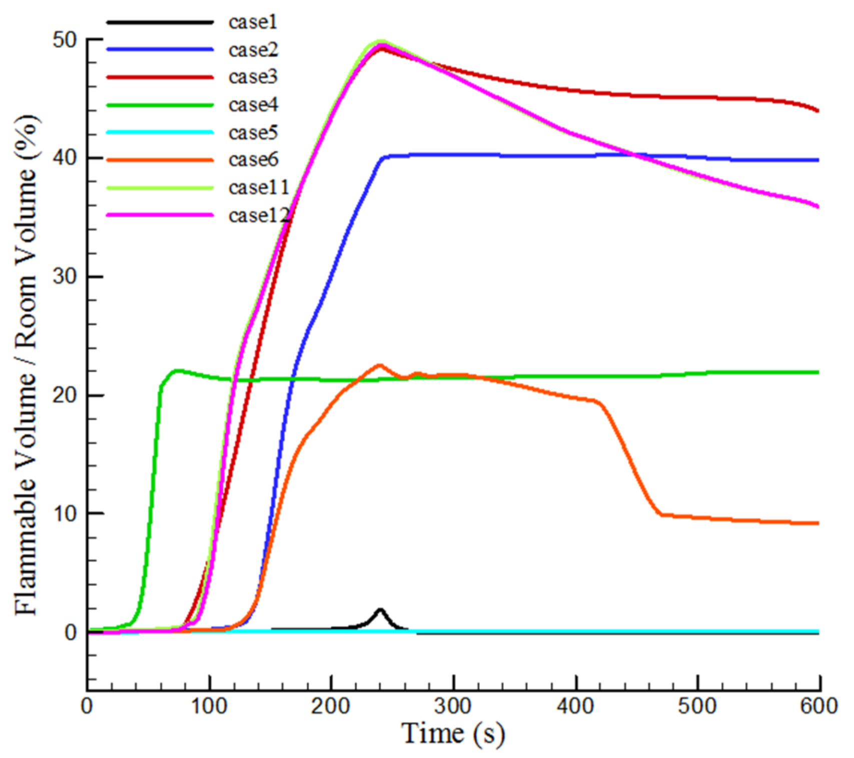


Figure 16. Flammable charge volume vs. time for Cases 1-6, 11, and 12 (FLUENT results)

4.2 CALIBRATION TESTS

To calibrate the proposed CFD models, tests were performed to study the release of flammable refrigerants into a single room for different scenarios and operating conditions. The tests were performed at Jensen Hughes in Baltimore, MD. The refrigerant used during the tests was R-32 (HFC-32, difluoromethane). The tests involved variation in refrigerant charge, flow rate, release height, presence/absence of ventilation and presence/absence of obstacles. The effect of these variables on refrigerant concentration was measured and documented for comparison to CFD predictions and calibration of the models. Details of the test enclosure, refrigerants, instrumentation, test procedure and results (including raw data) are given in the draft report prepared by Jensen Hughes on September 6, 2017: ***Flammable Refrigerant Dispersion Tests + Appendix A.*** A summary of the report is provided in this section.

4.2.1 Proposed test matrix and test enclosure

To collect adequate calibration data, the test matrix in Table 11 was developed by ORNL and proposed to Jensen Hughes (the tests were identical to the initial single room simulations for the wall-mounted AC in Table 10). As with the simulations, the baseline refrigerant charge for the calibration tests were based on the maximum charge limit equations found in IEC 60335-2-40 [4], which was a function of the test enclosure size, leak height and LFL. The leak location coordinates correspond to those in Figure 17 which gives dimensions of the test enclosure used (identical to dimensions of room used for Scenario 1 simulations, Figure 2).

Table 11. Test matrix proposed by ORNL for calibration tests conducted at Jensen Hughes

Test #	Refrigerant charge [kg]	Leak time [min]	Leak rate [g/s]	Obstacles	Leak location (x, y, z)	Remarks	Leak volumetric flow rate [SLPM]
1	3.257	4	13.572	None	(0, 1.83, 1.8)	Baseline case	378
2	4.886	4	20.358	None	(0, 1.83, 1.8)	1.5 x higher charge	567
3	6.515	4	27.144	None	(0, 1.83, 1.8)	2.0 x higher charge	756
4	3.257	1	54.289	None	(0, 1.83, 1.8)	1 min fast release	1513
5	3.257	10	5.429	None	(0, 1.83, 1.8)	10 min slow release	151
6	2.172	4	9.048	None	(0, 1.83, 1.2)	Different leak height	252
7	1.842	4	7.675	None	(0, 1.83, 0.6)	Different leak height	214
8	3.257	4	13.572	None	(0, 1.83, 1.8)	Liquid leak	378
9	3.257	4	13.572	Boxes	(0, 1.83, 1.8)	10% occupied	378
10	3.257	4	13.572	Boxes	(0, 1.83, 1.8)	25% occupied	378
11	6.515	4	27.144	None	(0, 1.83, 1.8)	Constant ventilation	756
12	6.515	4	27.144	None	(0, 1.83, 1.8)	Start ventilation at 10% LFL	756

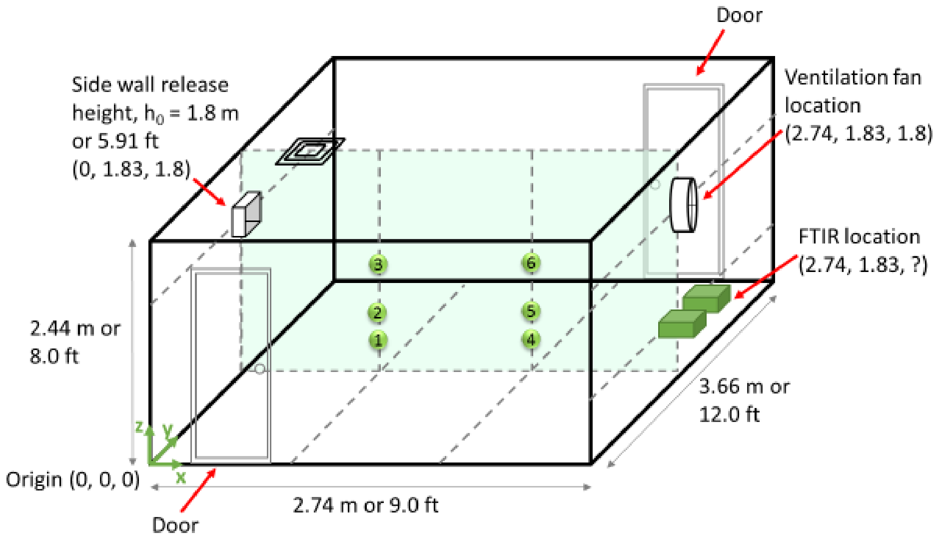


Figure 17. Test enclosure at Jensen Hughes, showing concentration measurement locations

As shown above, a nominal 2.7 x 3.7 x 2.4 m (9 x 12 x 8 ft) test enclosure was used for the refrigerant release testing. The suspended tile ceiling of the test enclosure was at an elevation of 2.4 m (8 ft) above the floor. The test enclosure was constructed with gypsum wall board over a metal stud frame. For a couple of tests, a ventilation system was added to the enclosure, consisting of an inline centrifugal duct fan with a capacity of 5,660 LPM (200 CFM). The fan was configured to draw from the test enclosure at a height of 1.8 m (6 ft) on the center of the western wall of the test enclosure. For a couple of tests, a second fan with a nominal capacity of 5,100 LPM (180 CFM) was mounted in box on the outlet of the diffuser. The box had holes drilled in the top and bottom to allow room air to mix with the refrigerant flow and avoid any pressurization of the diffuser due to the operation of the fan.

Cardboard boxes (12 x 12 x 12 in) were arranged inside the test enclosures to represent two different levels of obstacles (furniture and other clutter). A total of 86 boxes were added to represent 11% of the total volume and 196 boxes were added to represent 25.1% of the total volume, corresponding to tests 9 and 10 from Table 11, as shown in Figure 18. The layout is somewhat different than shown in Figure 3 (c and d) because the boxes available to JH were a bit larger than 0.305 m × 0.305 m × 0.305 m.

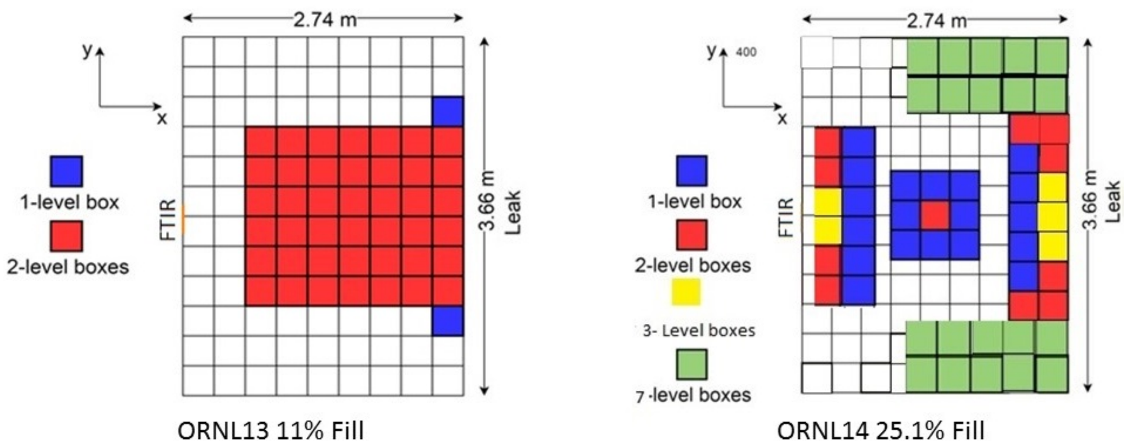


Figure 18. Obstruction locations for calibration tests 9 and 10 at Jensen Hughes

4.2.2 Instrumentation

The refrigerant was discharged from two steel cylinders through copper and stainless steel flexible tubing, terminating in a square duct diffuser that penetrated the enclosure wall. The diffuser duct was designed to make the refrigerant flow more uniform (as opposed to a concentrated jet) and was fabricated with three successively smaller perforated screens to reduce the refrigerant velocity. The flow of the refrigerant was controlled by a mass flow controller. The refrigerant release apparatus and diffuser assembly are shown in Figure 19.

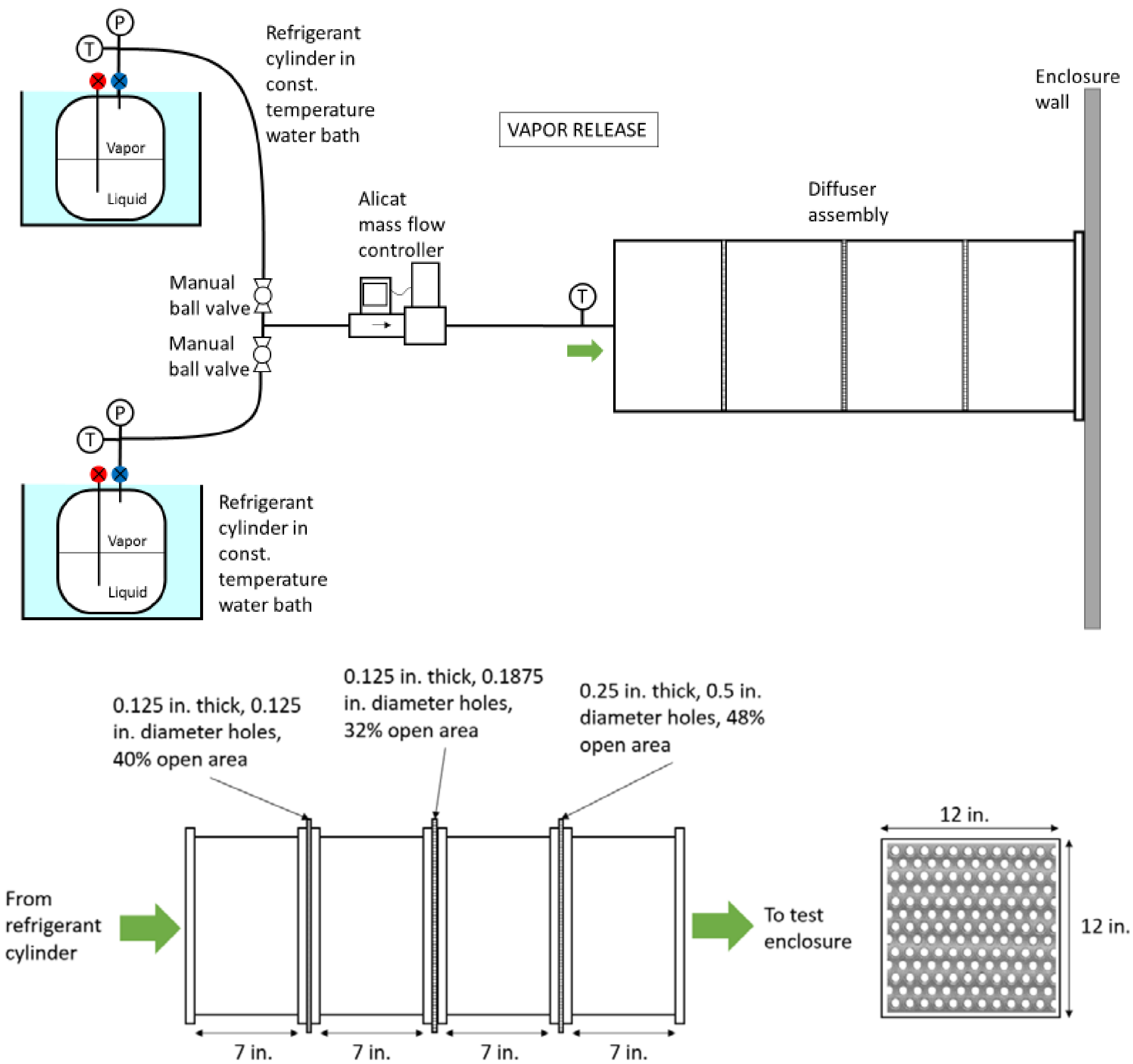


Figure 19. Refrigerant release apparatus and diffuser assembly for calibration tests at Jensen Hughes

For the tests involving liquid release and very high flow rate, a Coriolis flow meter and metering valve were used to measure and control the flow of refrigerant instead of the mass flow controller. In addition to the flow control and measurement, the other quantities that were measured were refrigerant temperature (in tubes prior to leak and at diffuser exit), air temperature at various locations in the test enclosure and refrigerant saturation pressure in the cylinders.

4.2.2.1 Concentration measurements

Two Tri-point Instruments, Model 123, dual gas analyzers were utilized to monitor the refrigerant concentration at six locations as illustrated in Figure 17. The analyzers worked on a thermal conductivity method and withdrew a continuous gas sample from three locations for analysis. The resolution was approximately 0.19% by volume with a range of 0- 34% for the R-32 refrigerant that was tested. The analyzer accuracy was ± 2% of full scale. The analyzers were calibrated to measure the refrigerants tested with a nominal 10% by volume mixture of the refrigerant and nitrogen in a cylinder. This represented a ±2.5% error on the scaling factor applied. The overall accuracy (meter and scaling factor) was approximately ± 4.6% of full scale.

The six sampling points were arranged in two vertical trees along the centerline of the enclosure. The trees were evenly spaced from each other and the sampling points were at elevations of 0.3, 0.9 and 1.5 m (1, 3 and 5 ft) above the floor.

A KVB Analect Diamond 20 Fourier Transform Infrared (FTIR) device with an external MCT detector was utilized to monitor the refrigerant concentration in the test enclosure in addition to the tripoint analyzers. The refrigerant concentrations were quantized by comparison with acquired spectras of known concentrations. The FTIR measurement beam was located across the center-line of the southern wall of the test enclosure at a height of 0.6 m (2 ft) at distance of 0.15 m (6 in) from the wall.

4.2.3 Test procedure

Prior to the start of a test, the test enclosure was configured as desired and the laboratory ambient conditions were recorded. The test enclosure configuration consisted of setting up the ventilation (if needed), arranging the cardboard box obstructions (if needed), installing the diffuser at the desired height and filling the discharge cylinder with refrigerant. The thermal conductivity analyzer zeros were then checked and the FTIR background obtained.

The data acquisition system, FTIR and the thermal conductivity analyzers were started, and after one minute of background data collection, the refrigerant was discharged into the test enclosure. The instrumentation was monitored for a minimum of fifteen minutes beyond the start of the refrigerant discharge. At the conclusion of the test, the test enclosure was purged with fresh air.

4.2.4 Summary of Jensen Hughes test results

A total of 21 tests were conducted, covering the 12 refrigerant discharge scenarios, and data were successfully obtained on the diffusion and mixing of refrigerant R-32 when released into an enclosure. Test 1 was the baseline case for use as a comparison for evaluating the effects of variables such as the height of the release point in the enclosure, refrigerant flow rate, discharge duration or total mass released, phase of the refrigerant (liquid or vapor) during the release, presence of obstructions and presence of operating ventilation. Although these represented a limited parametric evaluation, the data obtained were sufficient for model calibration purposes. The most critical data were obtained from measurements of refrigerant concentration as a function of time and at various locations in the enclosure. Example refrigerant concentration data for test 1 are shown in Figure 20. The concentration measurements were compared to the CFD model predictions, which were adjusted to align with experimental data.

The results showed that the increased refrigerant release amount resulted in increased refrigerant concentrations as expected. As the discharge time was held constant over this increased release, the refrigerant flow rate was increased. The increased refrigerant flow rate resulted in less of a concentration gradient in the enclosure. The liquid phase release, at the same flow rate, resulted in a steeper gradient corresponding to the lower temperature of the refrigerant flow after flashing to vapor in the diffuser and enclosure and the corresponding greater density of the flow.

The elevation of the release location was varied and was observed to result in higher concentrations below the release point and reduced concentrations above the release point with the release point lowered toward the floor. The presence of obstructions within the enclosure was found to increase the concentrations low in the space beyond that accounted for by the occupied volume of the obstructions. The reason for this was the effect the obstructions had on the mixing of the refrigerant within the enclosure.

The operating ventilation fan was located at the same height as the refrigerant release point for most of the tests. Since the refrigerant concentration at higher elevations was relatively low, and there was a make-up air vent in the suspended ceiling of the enclosure, the results showed that the ventilation had little effect on the refrigerant concentration for most of the tests. Overall, the experimental results provided valuable insights into the effects that various parameters had on refrigerant concentration and enabled accurate calibration of the CFD models, as discussed below.

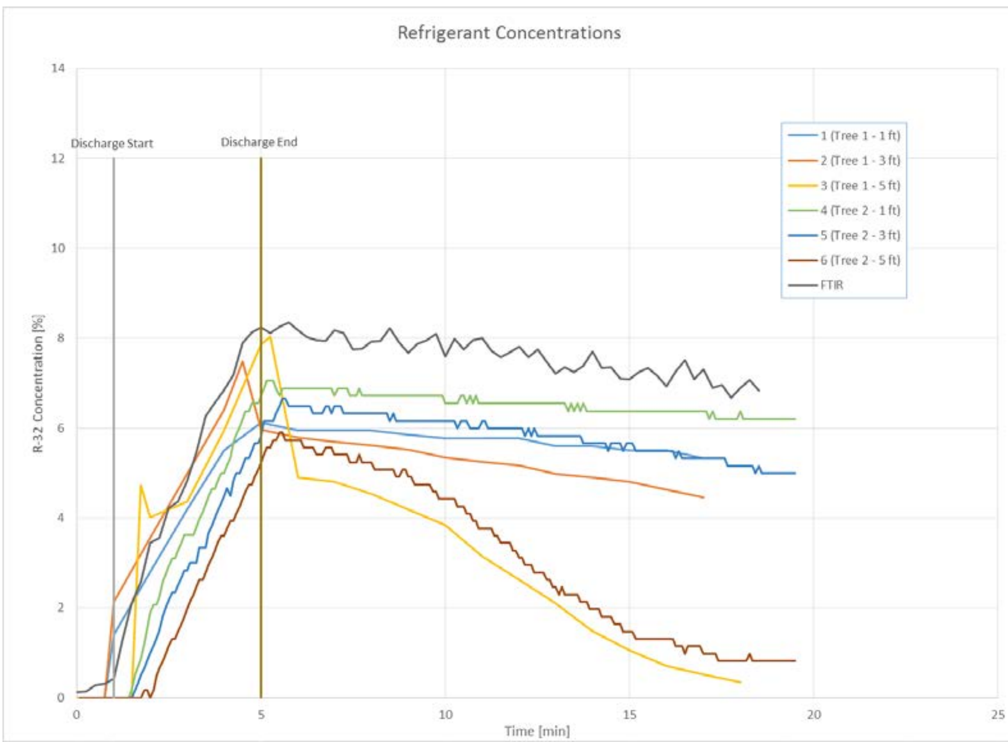


Figure 20. Refrigerant concentration data for Case 1 (baseline case) measured during calibration tests at Jensen Hughes

4.2.5 CFD calibration results summary

Comparing experimentally measured concentration gradients in Figure 20 with the initial simulation results at similar conditions in Figure 5 indicates that less charge stratification was observed than initially predicted by the models. As mentioned above, the leak was applied as a uniform mass-flow boundary condition across the return air grill in the initial simulations resulting in a low-momentum cascade of refrigerant exiting the grill and flowing to the floor producing the high concentration gradients. However, observations of the leak release during the calibration testing at Jensen Hughes and during shakedown testing of the release duct system at ORNL indicated that the refrigerant actually left the release control system and entered the test room as a relatively high momentum plume (Figure 21). Therefore, several approaches were tested in CONVERGE to develop a more accurate representation of the observed leak release pattern.

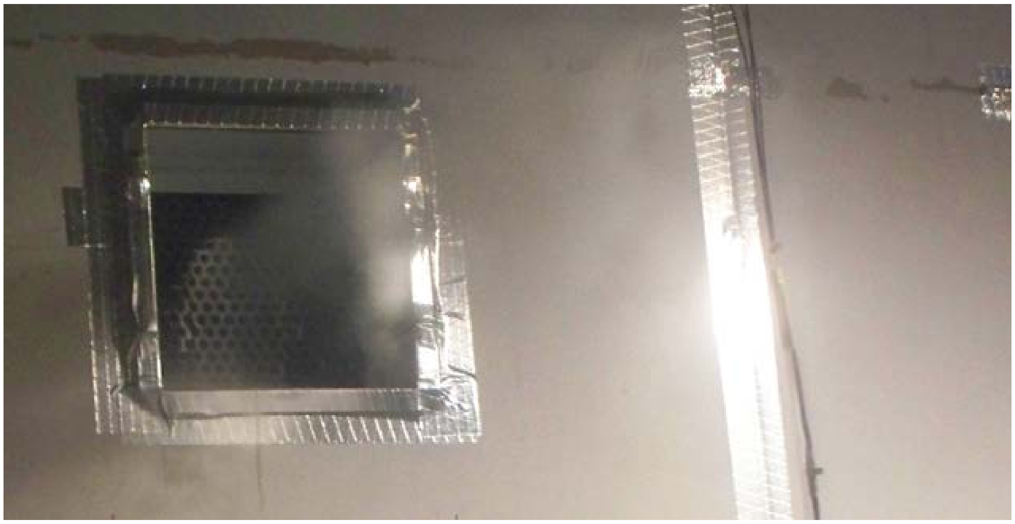


Figure 21. Refrigerant release pattern (for Case 8, liquid release) observed during calibration testing at Jensen Hughes

Initial efforts involved modeling the geometry of the leak point and ductwork used to introduce the refrigerant to the room in the experimental study (Figure 19). However, as shown in Figure 22, this approach also predicted a low-momentum cascade of refrigerant exiting the duct.

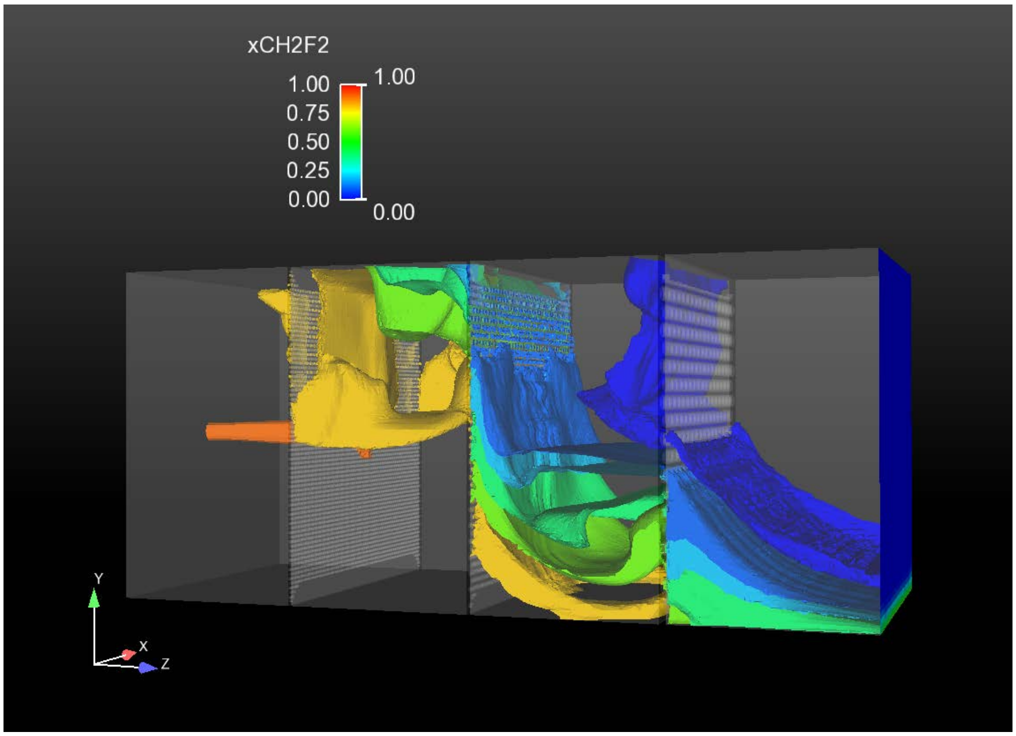


Figure 22. CONVERGE simulation of R-32 point leak progressing through the release duct used in the calibration testing; refrigerant exit at right-hand side (low momentum, water fall at duct exit)

As a second attempt, we simply varied the area through which the leaked refrigerant enters the room using a square grid ranging in size from 0.305 m to 0.001 m equivalent diameter. It was determined that a release grid of ~25 mm (1 inch) equivalent diameter produced the best match. As shown in Figure 23 below, the resulting simulated concentration profile (solid lines) matched the test results (dashed lines) within the experimental uncertainty band (about ±4.5%). The trend was similar for the other cases (results are not shown here).

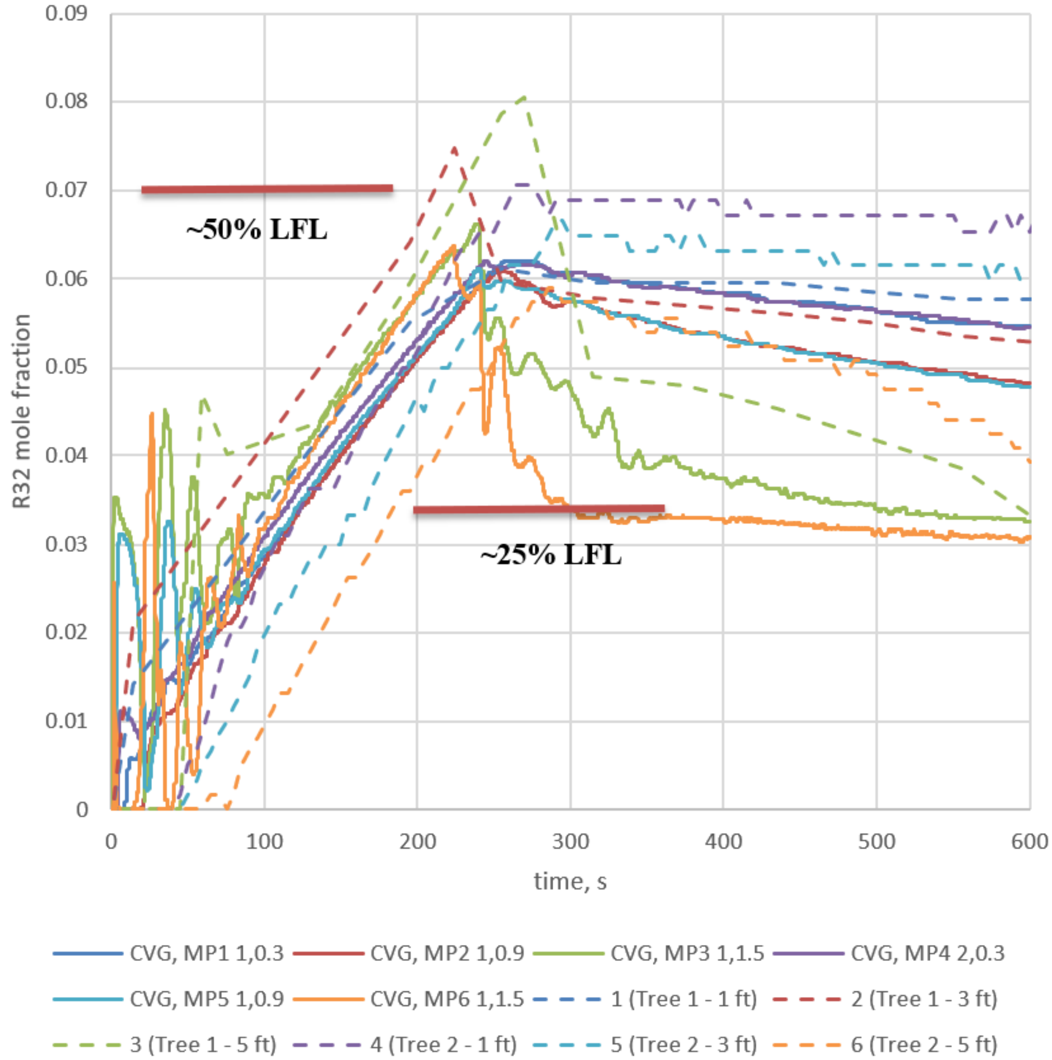


Figure 23. Experimental and numerical data for Case 1 at different monitor points

4.3 SIMULATION OF MULTI-ROOM RESIDENCE WITH PACKAGE AC UNIT

4.3.1 Case setup

The second group of simulations focused on the leak from a 10.55 kW (3-ton) package AC unit (16 SEER, 3.175 kg (7 lb) charge) connected to duct system serving a 167.23 m^2 (1800 ft^2) 4-room residence (Figure 24 below).

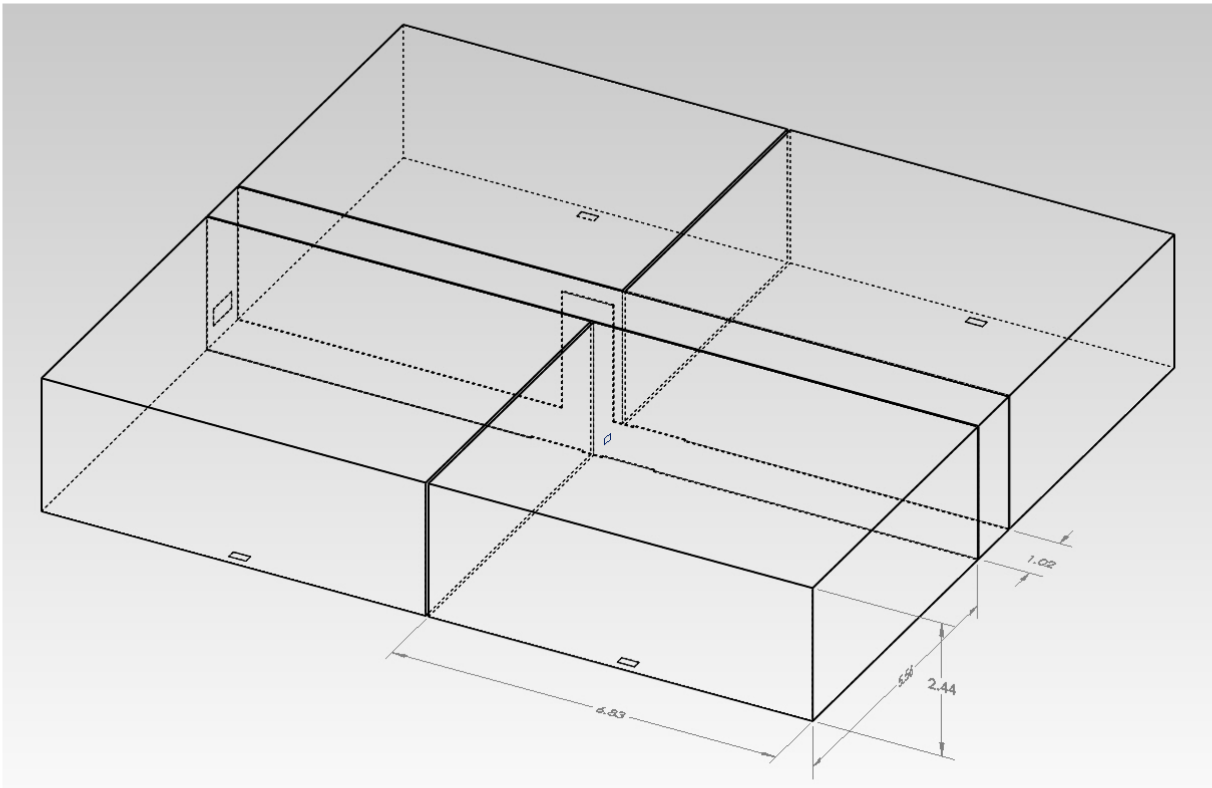


Figure 24. 4-room residence configuration for Case 9, Table 12, one door open (dimensions in meters)

A total of nine cases were simulated with two refrigerants, R-32 and R-452B. Both floor and ceiling ducts were considered in the simulations. Two leak durations were simulated: a slow leak (4-min duration) and a very fast (catastrophic) leak. The catastrophic leak represented a total rupture of a 6.35 mm (¼”) pipe downstream of the evaporator coil. For this case, the leak flow rate (at the instant it starts) was calculated from the orifice equation as follows

$$v = C_d \sqrt{\frac{2\Delta P}{\rho}} \tag{3}$$

where C_d is the coefficient of discharge (0.8), ΔP is the pressure difference across the rupture and ρ is the refrigerant (R-32) density (for saturated vapor at 280 K (44.3 °F)). Using the above equation, the leak mass flow rate was computed to be 0.1786 kg/s (0.393 lb/s). For the saturation temperature assumed, the vapor velocity is ~206 m/s (~676 ft/s), giving a Mach number of ~0.98 based on the R-32 saturated vapor sonic velocity of ~209 m/s [24]. So, the CONVERGE CFD computations are based on its compressible gas flow solver as noted in Table 7 earlier. Using equation 3 for the leak flow and an incompressible gas flow solver for the flow field from that point forward might have provided similar results, but this has not been tested. Prior team experience with other flow field modeling using CONVERGE led us to choose the incompressible flow solver for the entire flow field for this project.

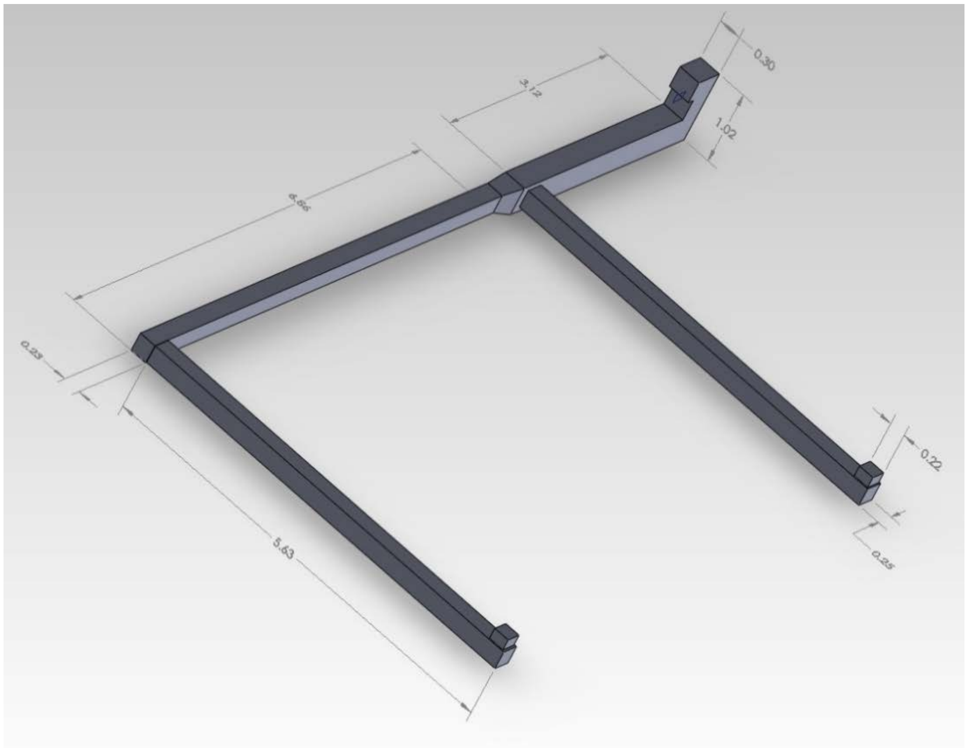
Table 12 presents the 9 simulated cases.

Table 12. Simulation parameters for 4-room residential space with package AC unit

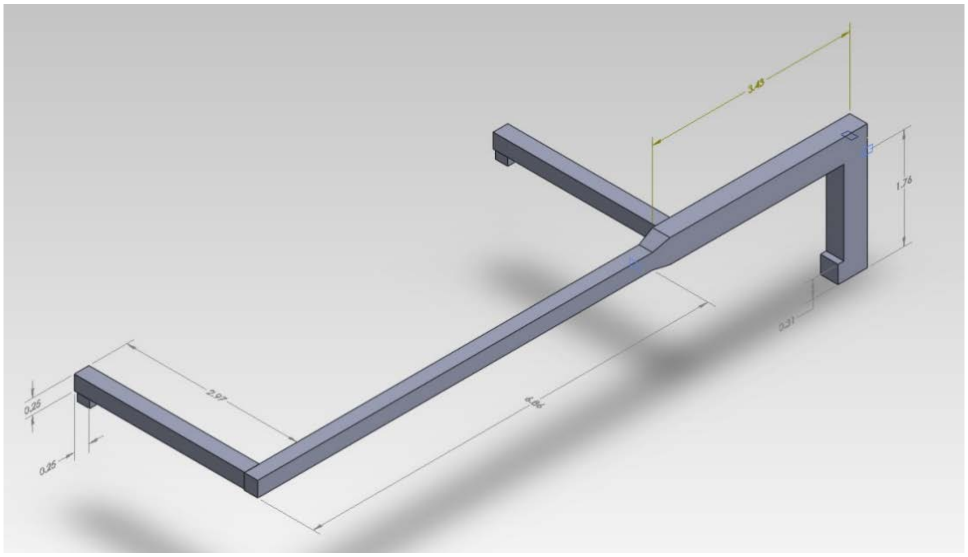
Test #	Refrigerant	Remarks[a,b]	Leak duration [s]
1	R-32	All rooms open Floor supply registers	240
2	R-32	All rooms open Ceiling supply registers	240
3	R-32	All rooms open Floor supply registers	17.8
4	R-452B	All rooms open Floor supply registers	240
5	R-32	All rooms closed Floor supply registers	240
6	R-452B	All rooms closed Floor supply registers	240
7	R-32	All rooms closed Floor supply registers	17.8
8	R-32	All rooms closed Floor supply registers Supply air fan on	17.8
9	R-32	Two rooms open & two closed Floor supply registers	17.8

[a]AC unit indoor fan assumed off for all cases except Case 8
[b]No duct leakage assumed for duct simulations

The need for high spatial resolution within the duct combined with the large volume of the multi-room residence presented a challenge for simulating this scenario with acceptable computational times. A work-around approach was chosen in which the duct and room were modeled separately with the duct simulation providing boundary conditions (flow rate and concentration) for the refrigerant entering the room. The duct simulations assumed no leakage from the duct to ambient (crawlspace or attic), and the AC unit indoor fan was off for all except Case 8. Figure 25 shows the ceiling and floor duct system design and dimensions. Both the duct and room designs were set up to be symmetrical allowing the simulations to be performed on half the total duct or space volume to further reduce computational time and resource needs (memory and number of cores). For the floor duct case the AC unit was assumed to be located below the house floor level (a crawlspace installation), and for the ceiling ducts an attic location was assumed.



(a.)



(b.)

Figure 25. Duct design for (a) floor duct and (b) ceiling duct (dimensions are in meters and half duct is shown)

4.3.2 Results

Figure 26 shows the predicted time history of flammable refrigerant/air volume inside the supply ducts for the standard leak cases with R-32 (left) and R-452B (right).

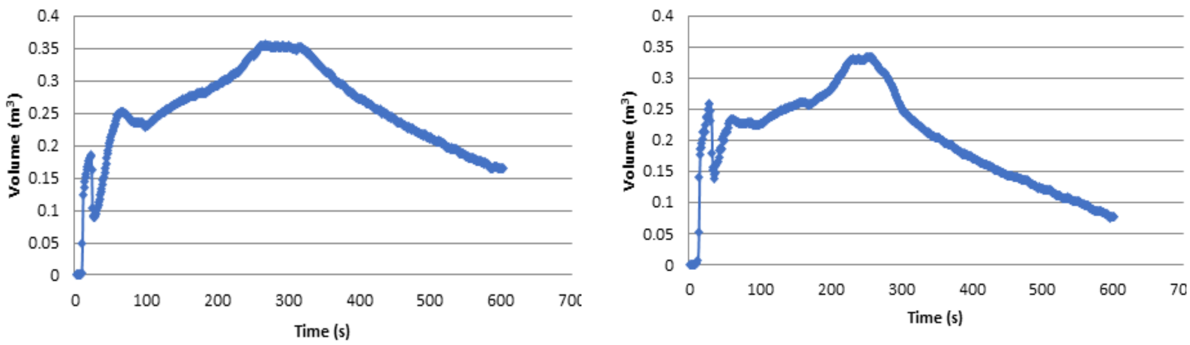
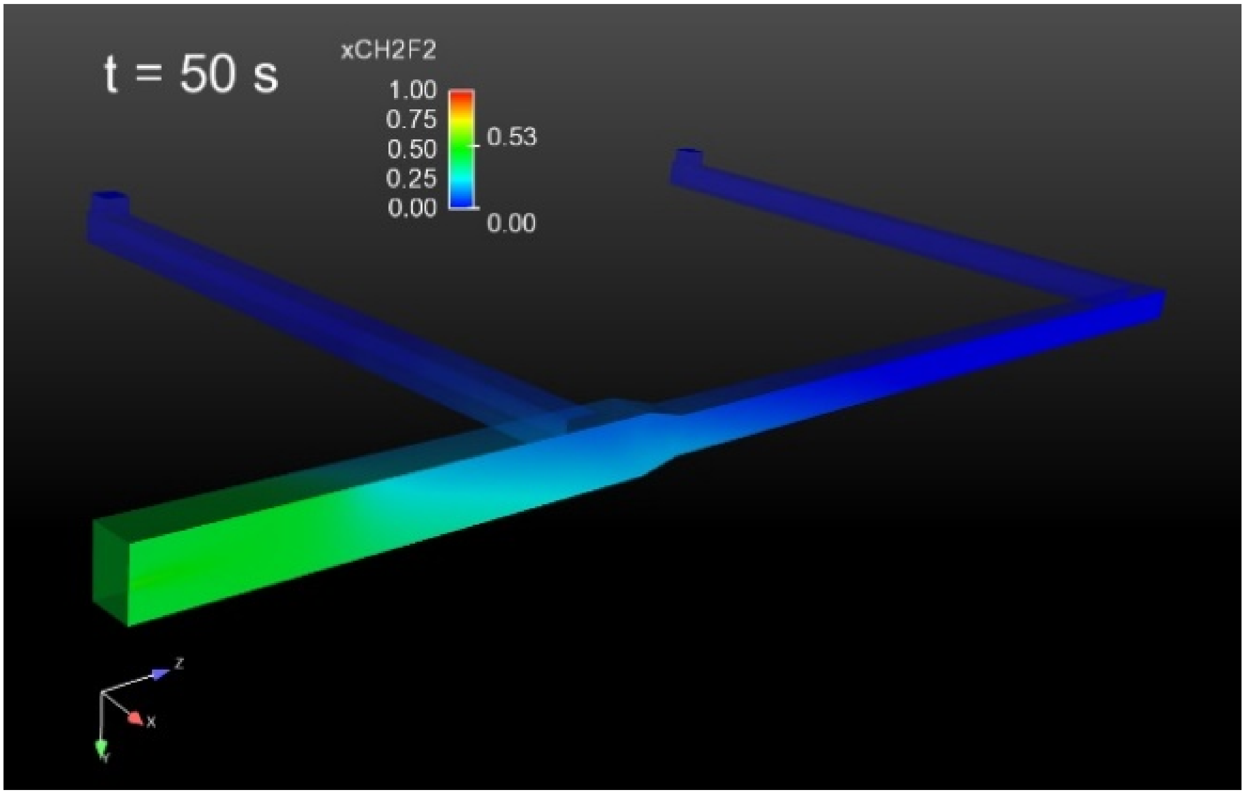
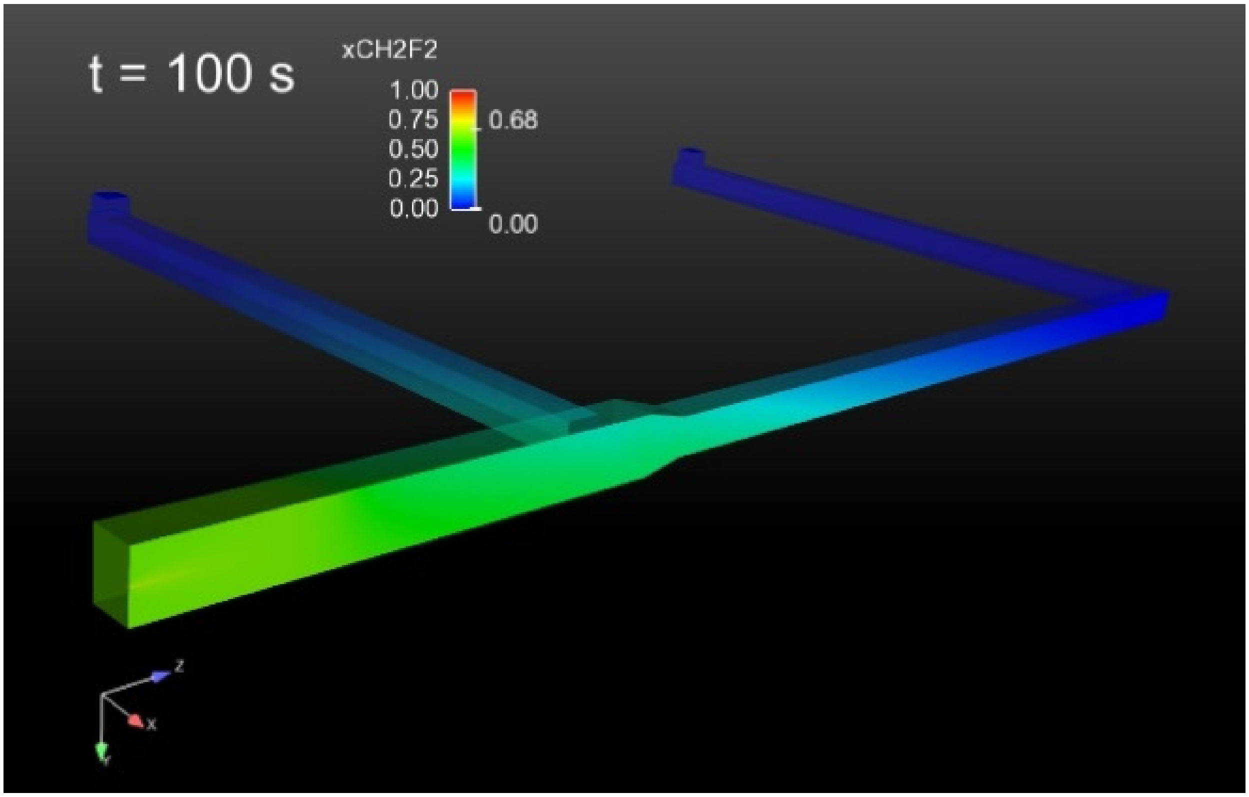


Figure 26. Flammable volume (refrigerant concentration between LFL and UFL) inside underfloor supply ducts vs. time for a 4-min leak with R-32 (Cases 1 and 5, left) and R-452B (Cases 4 and 6, right).

Figure 27 (for standard leak rate cases 1 and 5) shows that the refrigerant disperses through the duct very slowly. Concentrations remain high near the leak point longer due to the longer leak duration (240 s). After the leak ends (at the 240s point), diffusion through the duct occurs more slowly with concentrations at the outlets reaching a maximum of only 11% for the front room (outlet 1) and 22% for the back room (outlet 2) at the 10-min mark (end of simulation time period) with no measurable amount of refrigerant predicted to enter the rooms.

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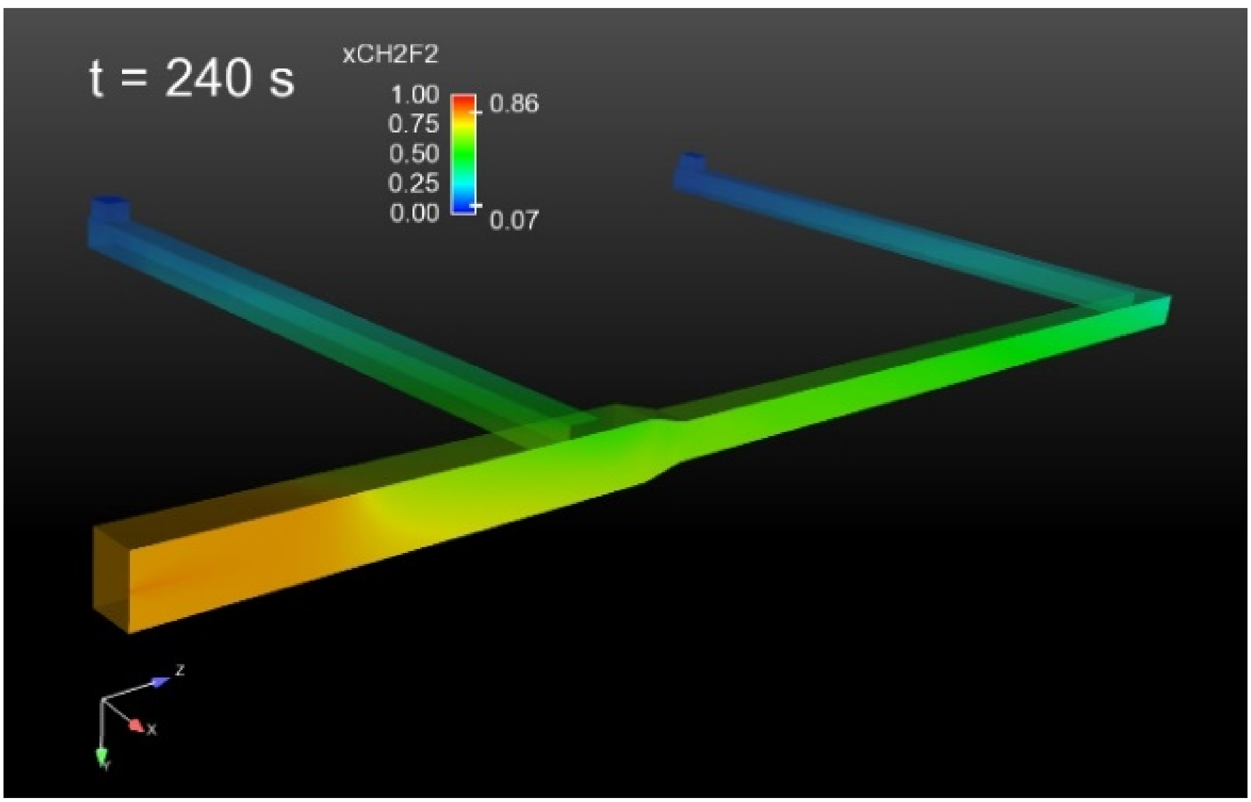
0.00
z
x
y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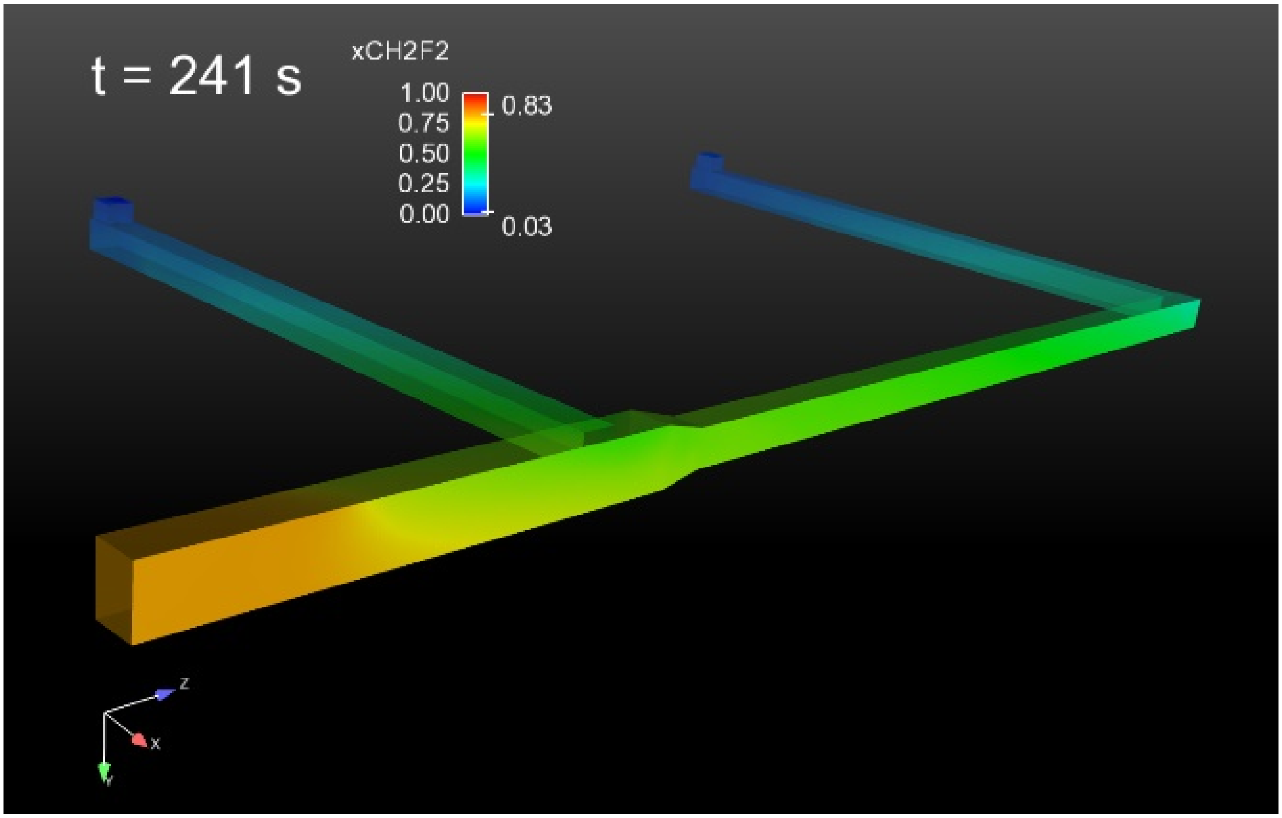
0.07
z
x
y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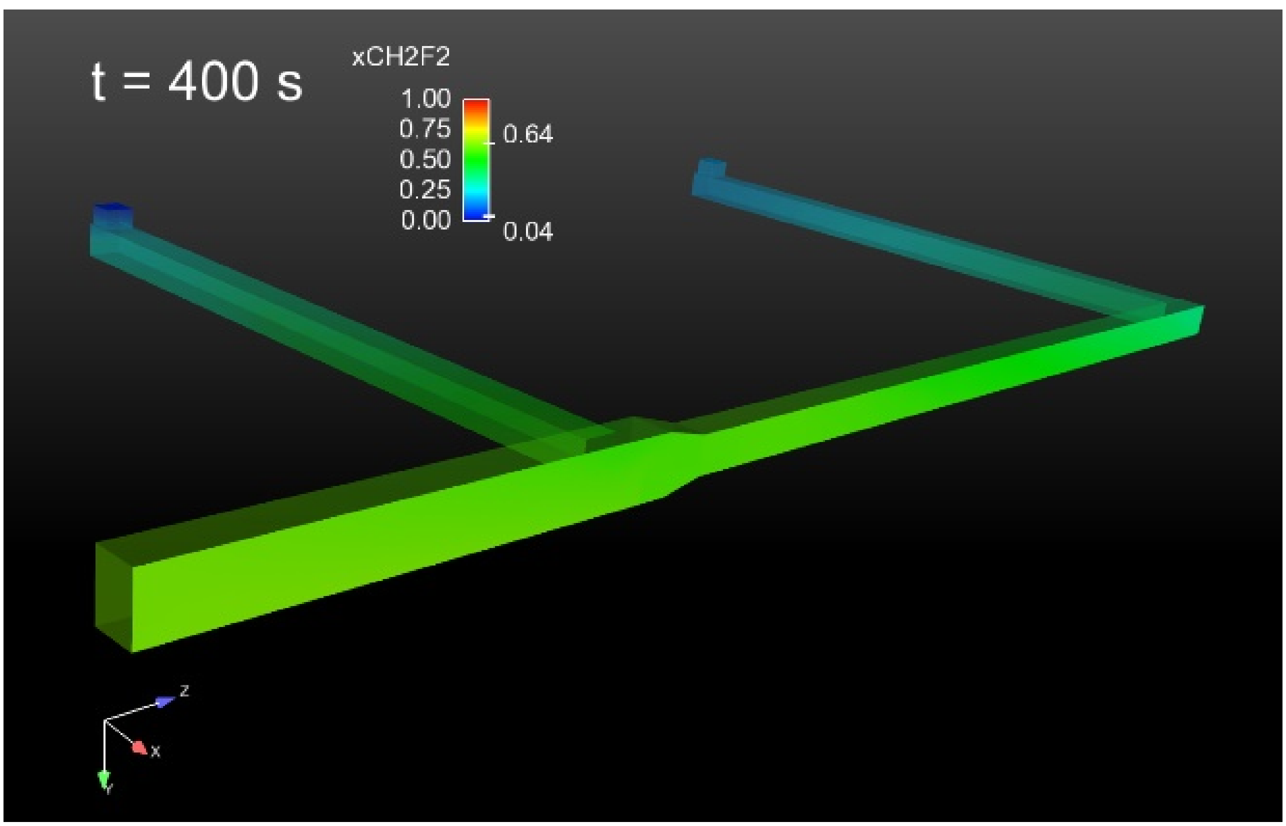
z
x
y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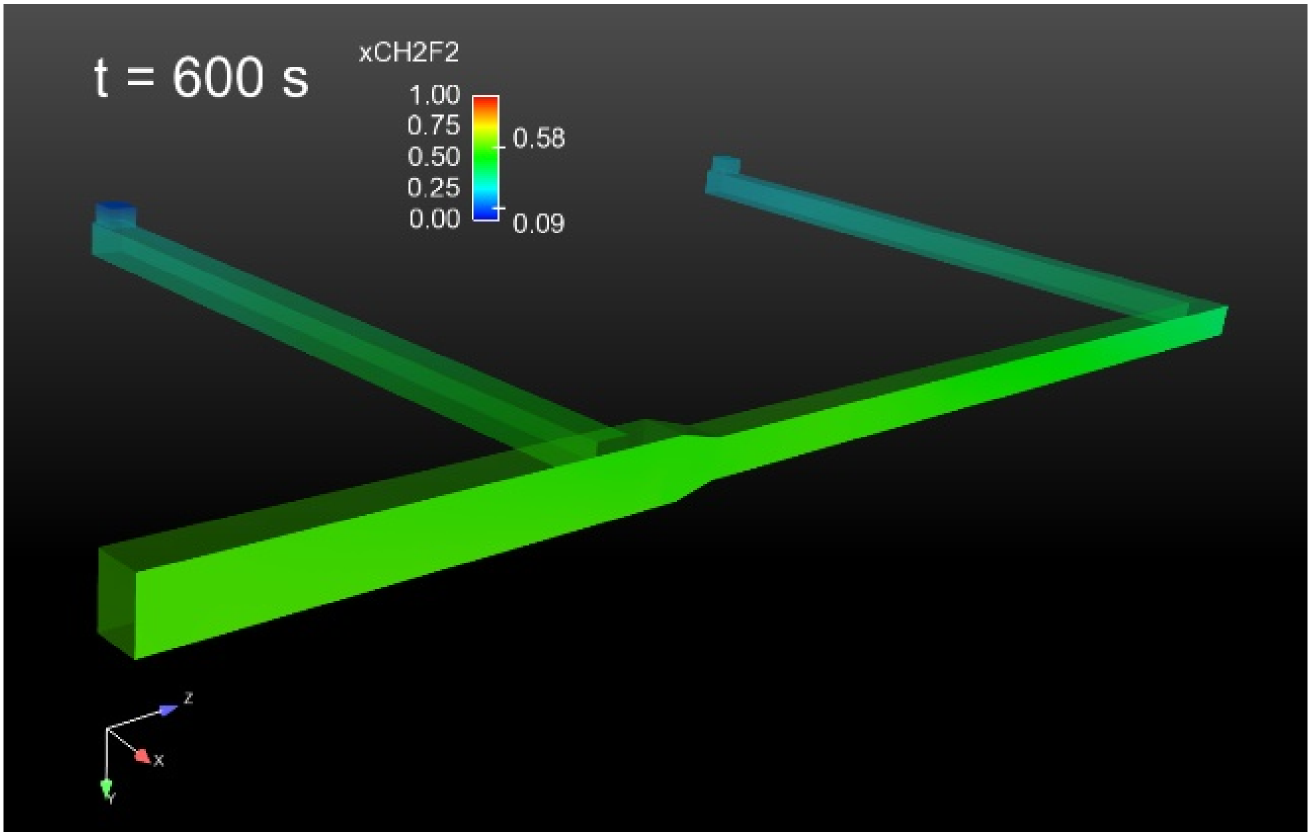
x
y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x
Y

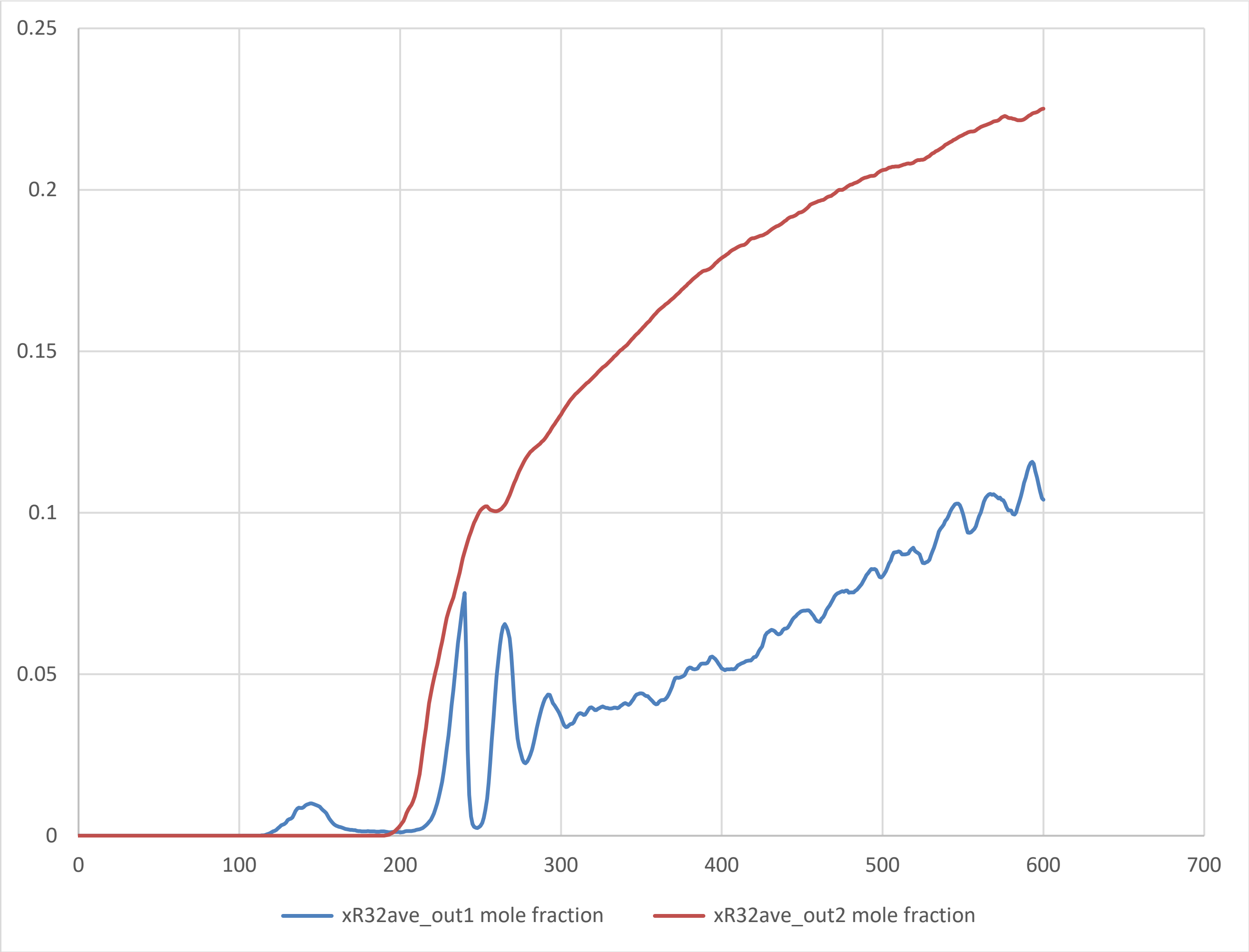
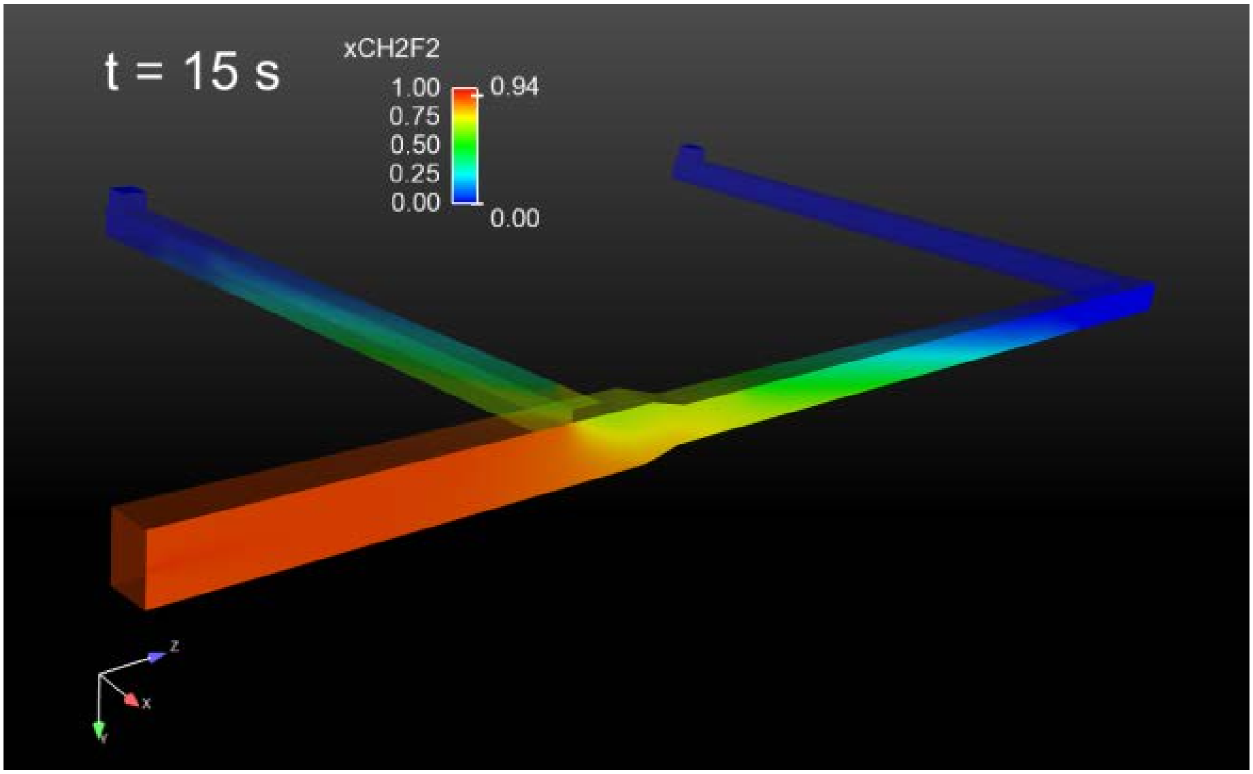
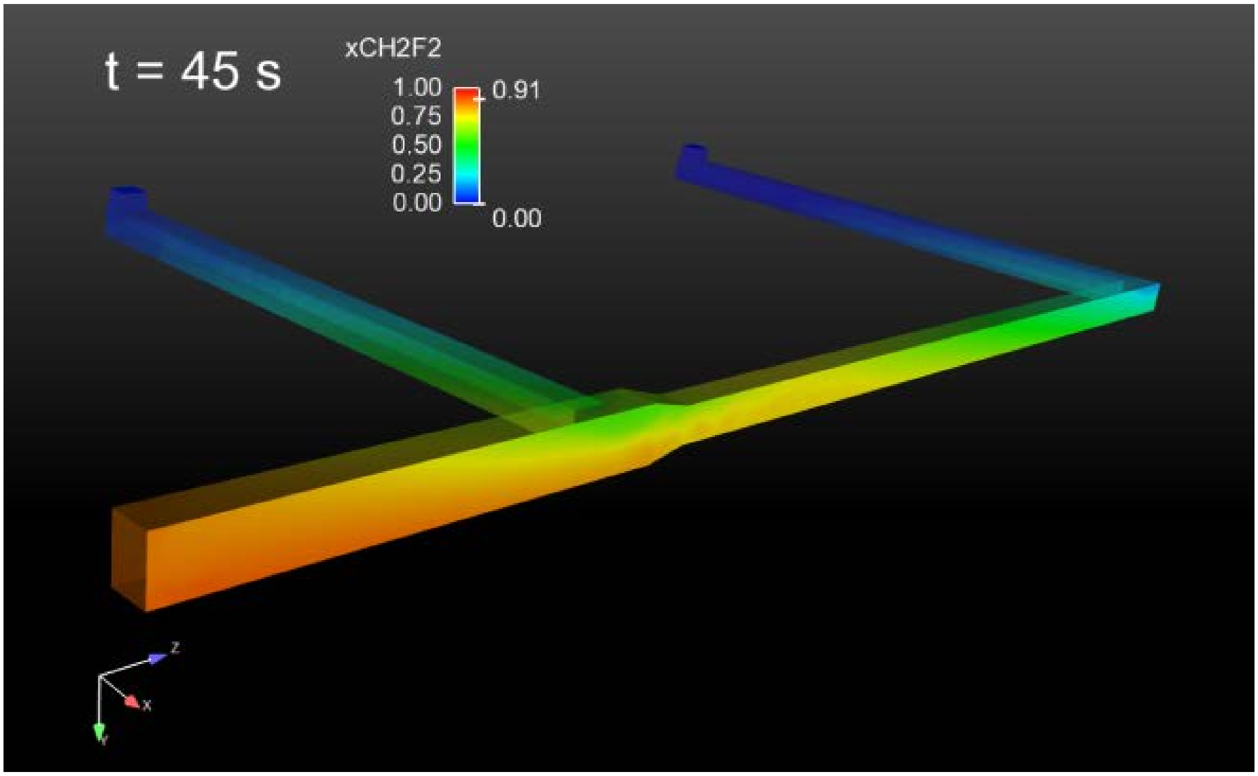


Figure 27. Contours of R-32 volume fraction in the floor duct at 50s, 100s, 240s, 241s, 400s, and 600s with plot of R-32 concentration vs. time at outlets 1 (blue line) and 2 (red line) for slow (4-min) leak cases 1 and 5

For the floor duct with fast leak of R-32 (cases 3, 7, and 9 in Table 12), Figure 28 shows that the maximum concentration is seen close to the leak source at the duct entrance. The momentum of the leaked refrigerant quickly drops resulting in a slow progression throughout the remainder of the ductwork. Concentrations remain high as the refrigerant moves through the duct displacing the lighter air upward out the floor vents rather than mixing with it. After the leak ends (at 17.8 s), the refrigerant continues to slowly disperse along the duct toward a uniform equilibrium within the flammability limits. While the concentration of refrigerant eventually reaches 23% at outlet 1 and 28% for outlet 2, due to its low momentum, only 19g of refrigerant is predicted to overcome gravity and enter the room through the floor grates leaving almost all of the refrigerant in the ductwork at flammable concentrations. This combination of high flammable volume within the confines of the ductwork represents a significant fire risk if an ignition point is introduced (e.g., sparking when the system fan turns on). Note that this represents a worst-case scenario since no leakage from the ducts to surrounding ambient was assumed for these simulations. In a real case it can be expected that the refrigerant remaining in the duct will eventually escape to the crawlspace or attic and disperse to the outdoors. Still, for a fairly tight, low-leakage duct system, the results indicate a significant likelihood that a flammable volume could persist inside the ductwork for an extended time. The risk could be reduced by including a refrigerant sensor in the AC unit coupled with controls to start the unit blower in event refrigerant concentration above a set point (e.g., >25% LFL or other) is detected.

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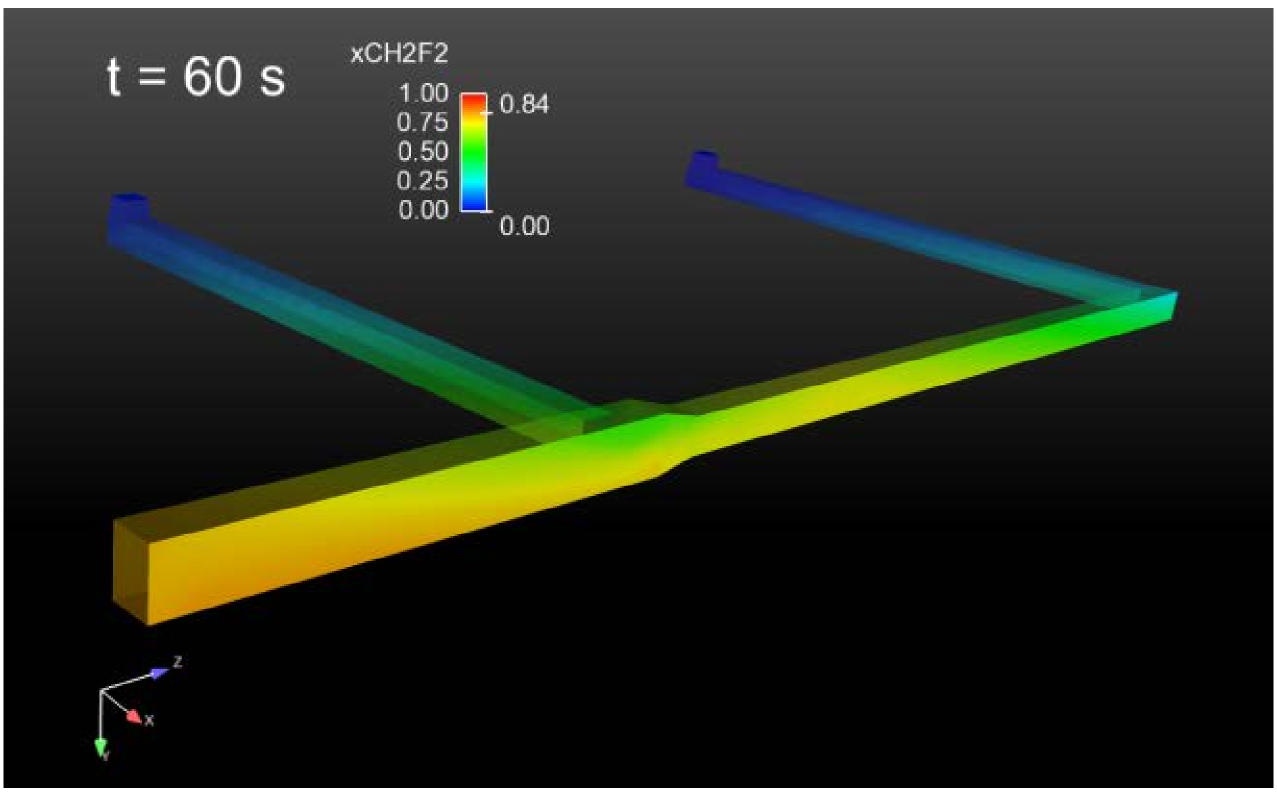
x
y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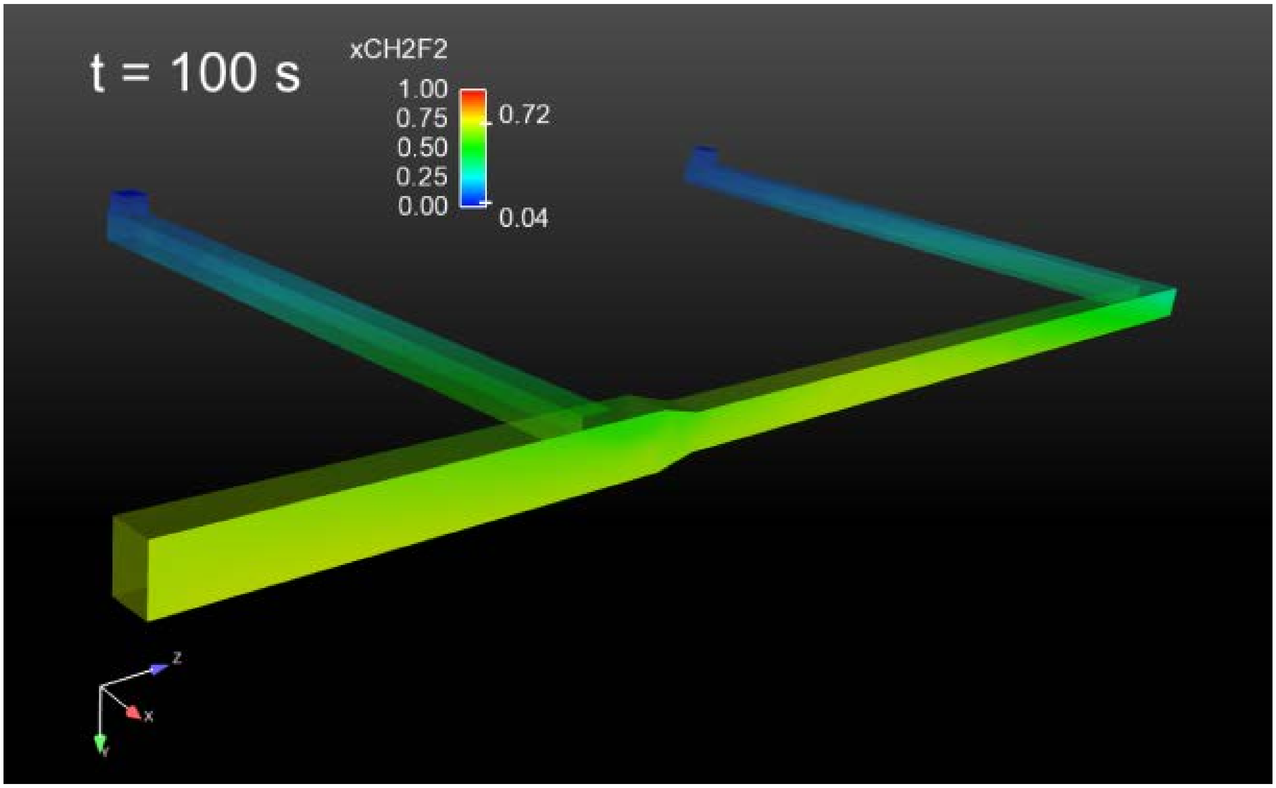
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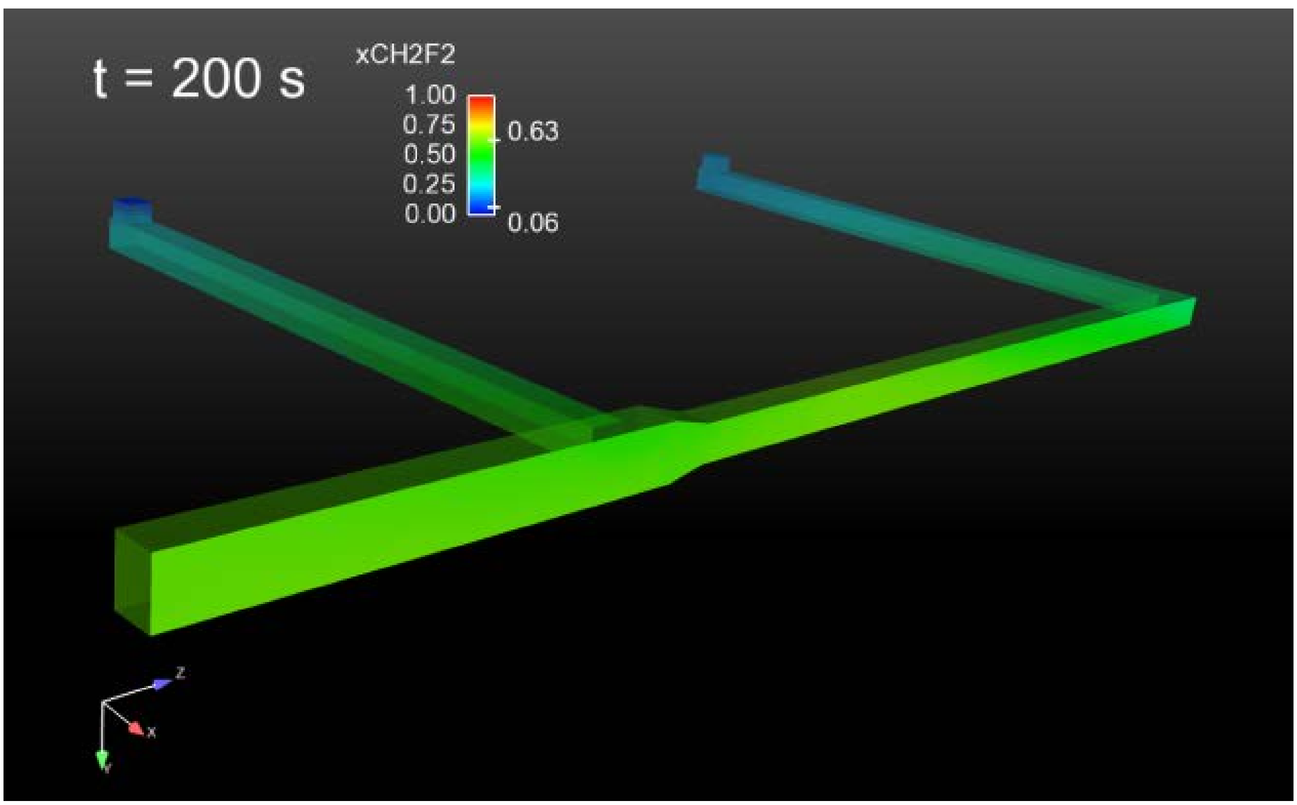
0.04
z
x
y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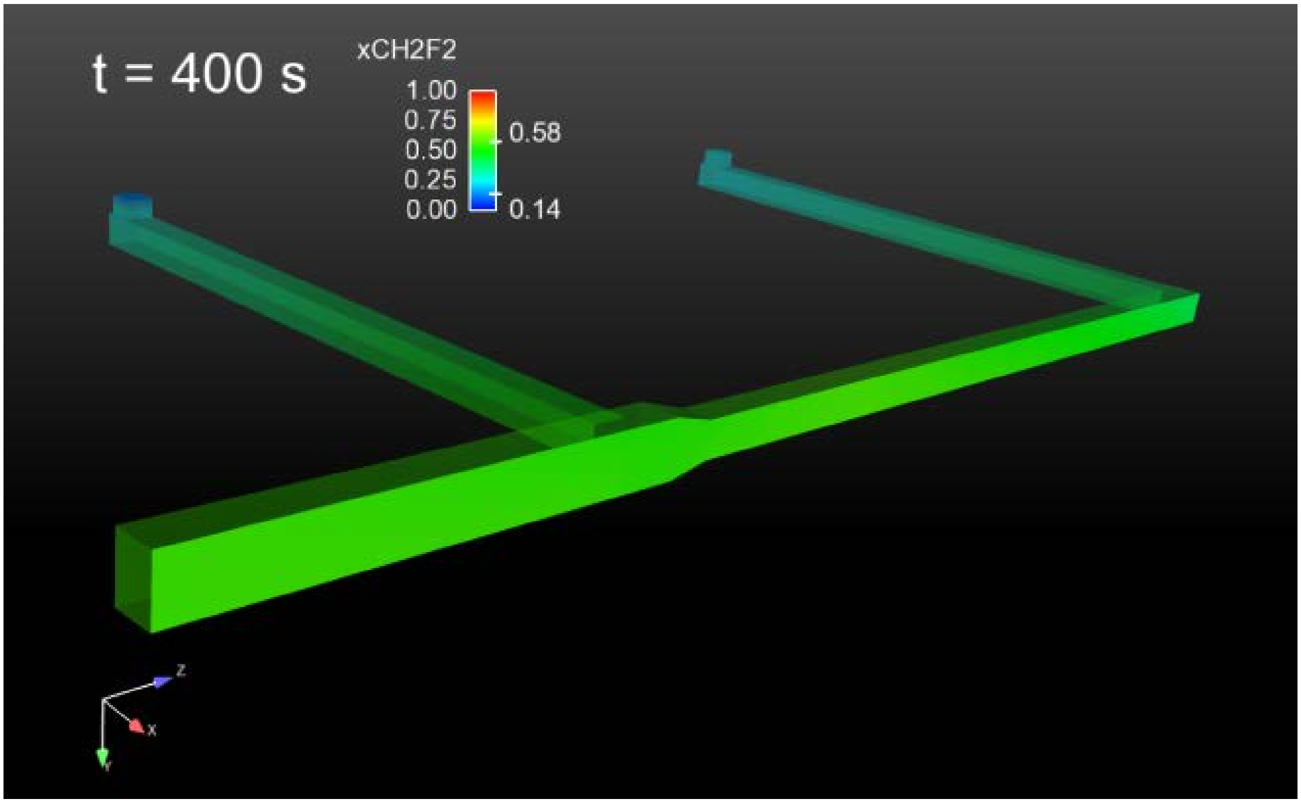
z
x
y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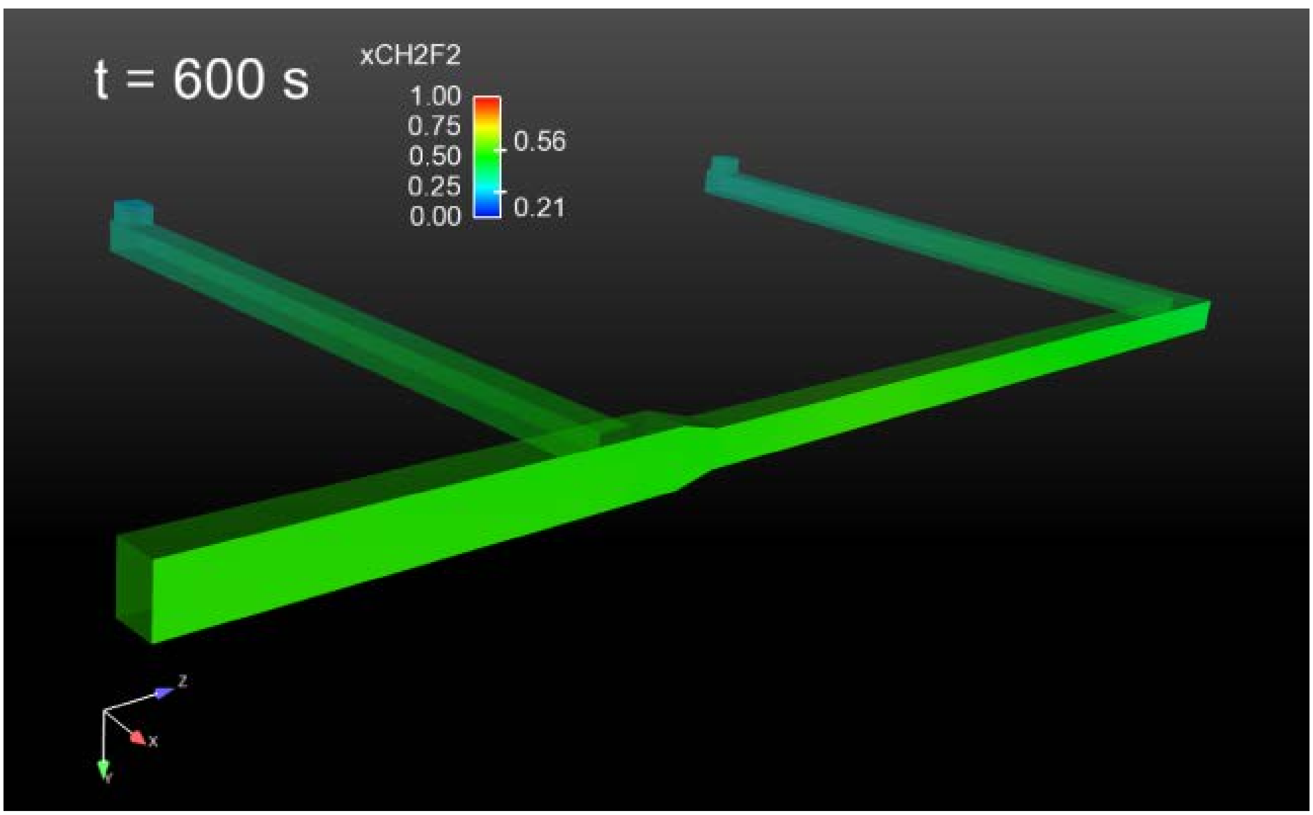
0.25
0.00
0.58
0.14
z
x
y


t = 600 s
xCH2F2
1.00
0.75
0.50
0.25
0.00
0.56
0.21
z
x
y

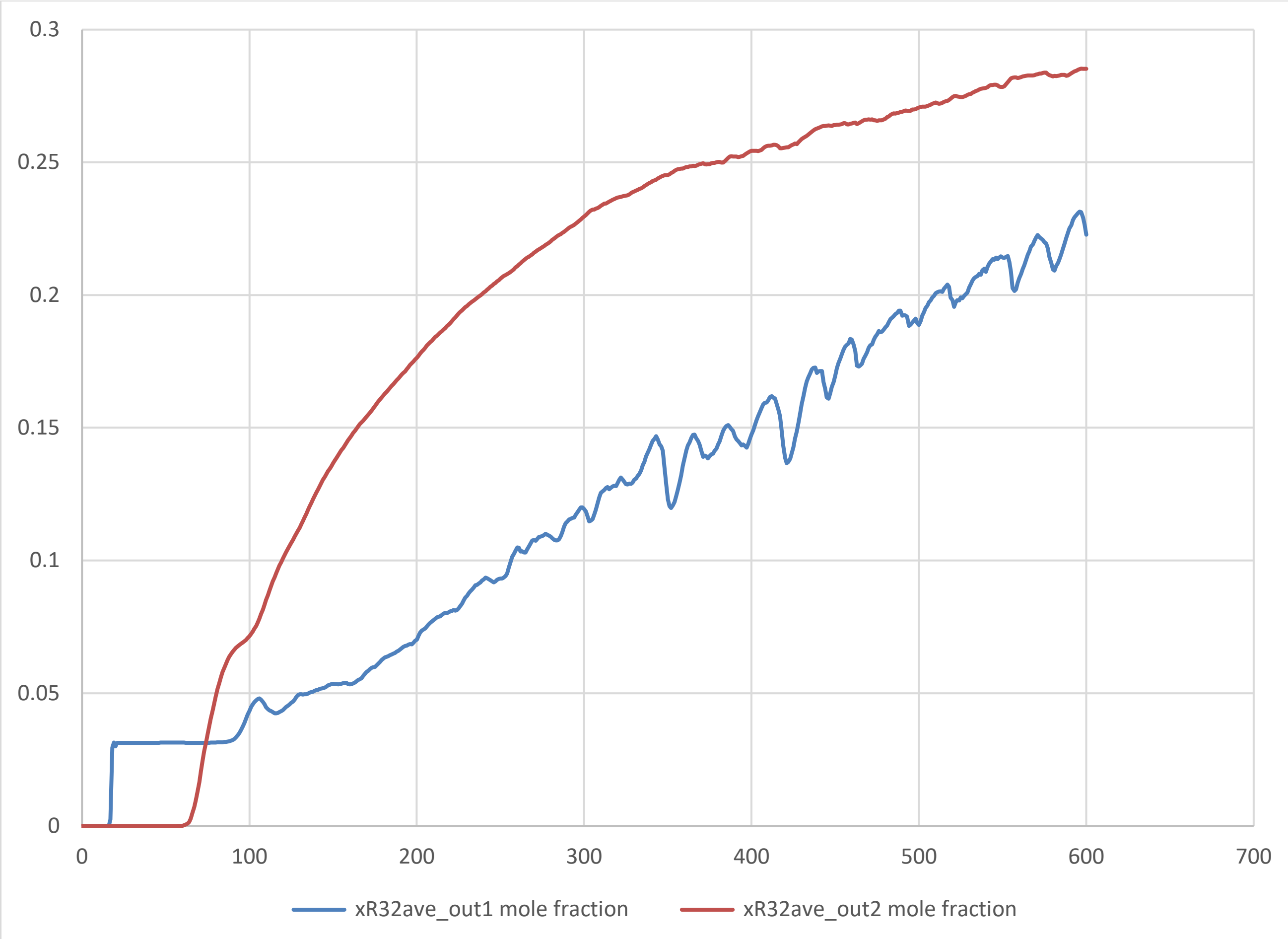
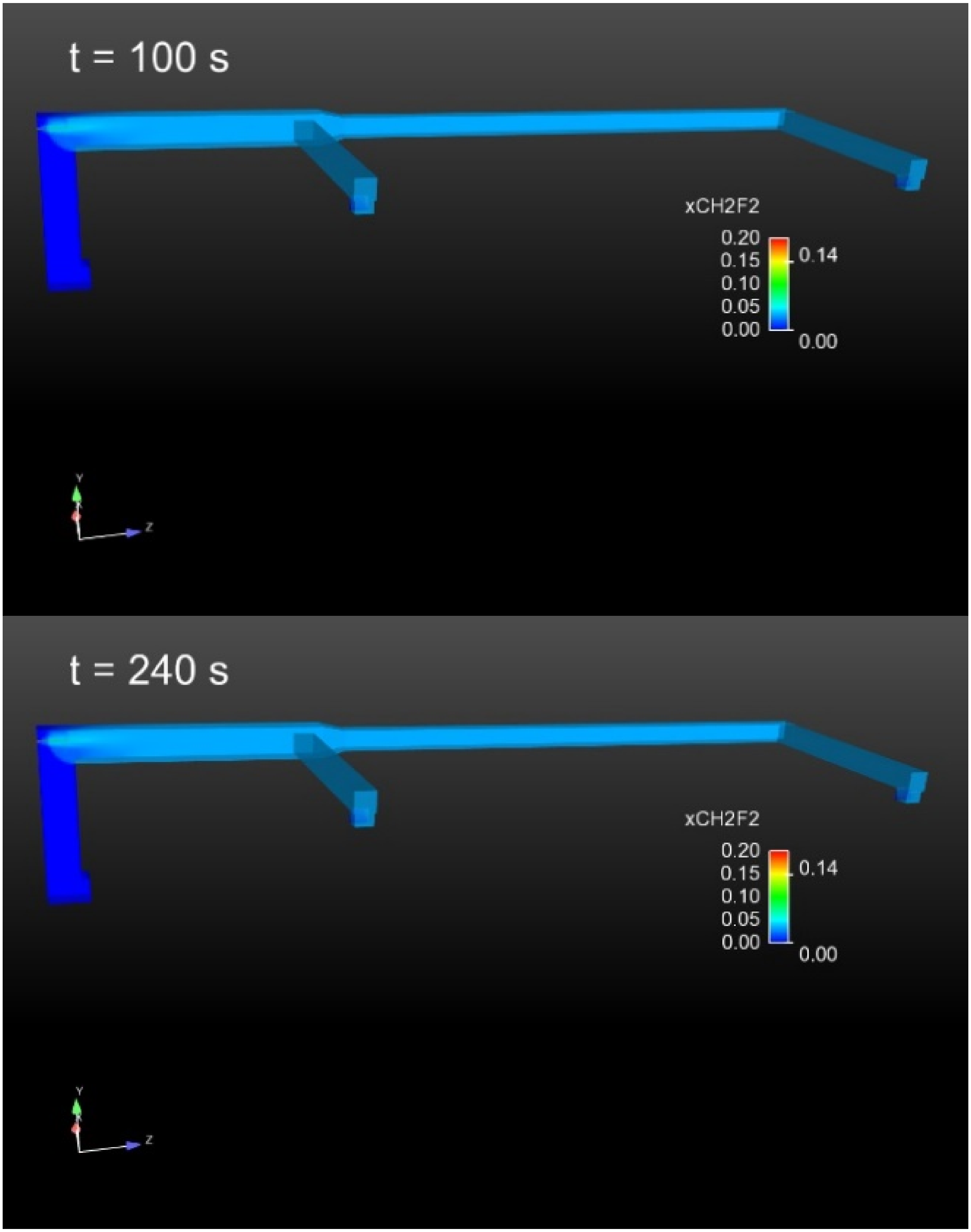


Figure 28. Contours of R-32 volume fraction in the floor duct at 15s, 45s, 60s, 100s, 200s, 400s, and 600s with plot of R-32 concentration vs. time at outlets 1 (blue line) and 2 (red line) for fast leak cases 3, 7, and 9

For the ceiling duct case 2 (Figure 29), gravity is no longer an obstacle to overcome and instead aids entry of the refrigerant into the room from the ductwork. The momentum of the leaking refrigerant draws air up through the return duct mixing with the refrigerant and lowering overall concentration levels as it moves through the ductwork. As a result of the mixing with air and quick transport of the refrigerant into the room, the mixture reaches a maximum predicted concentration of 14% within the duct which is slightly below the LFL concentration of 14.4%. When the leak ends at 240 s, the refrigerant still present in the duct quickly reverses direction and flows down and out the return duct. Within 16 s of the leak ending, all refrigerant has exited the duct.


t = 100 s
xCH2F2
0.20
0.15
0.10
0.05
0.00
0.14
0.00
Y
Z
t = 240 s
xCH2F2
0.20
0.15
0.10
0.05
0.00
0.14
0.00
Y
Z

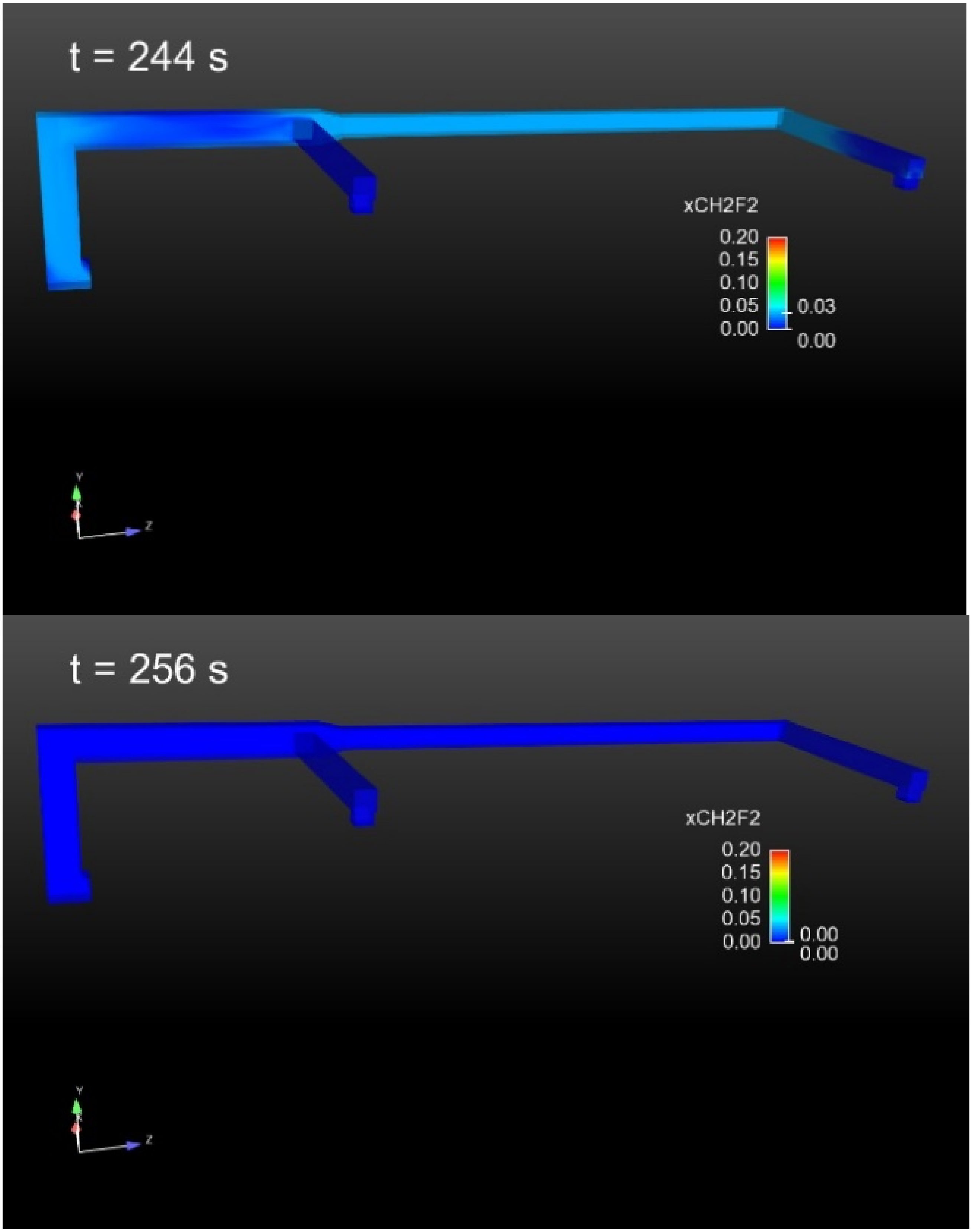
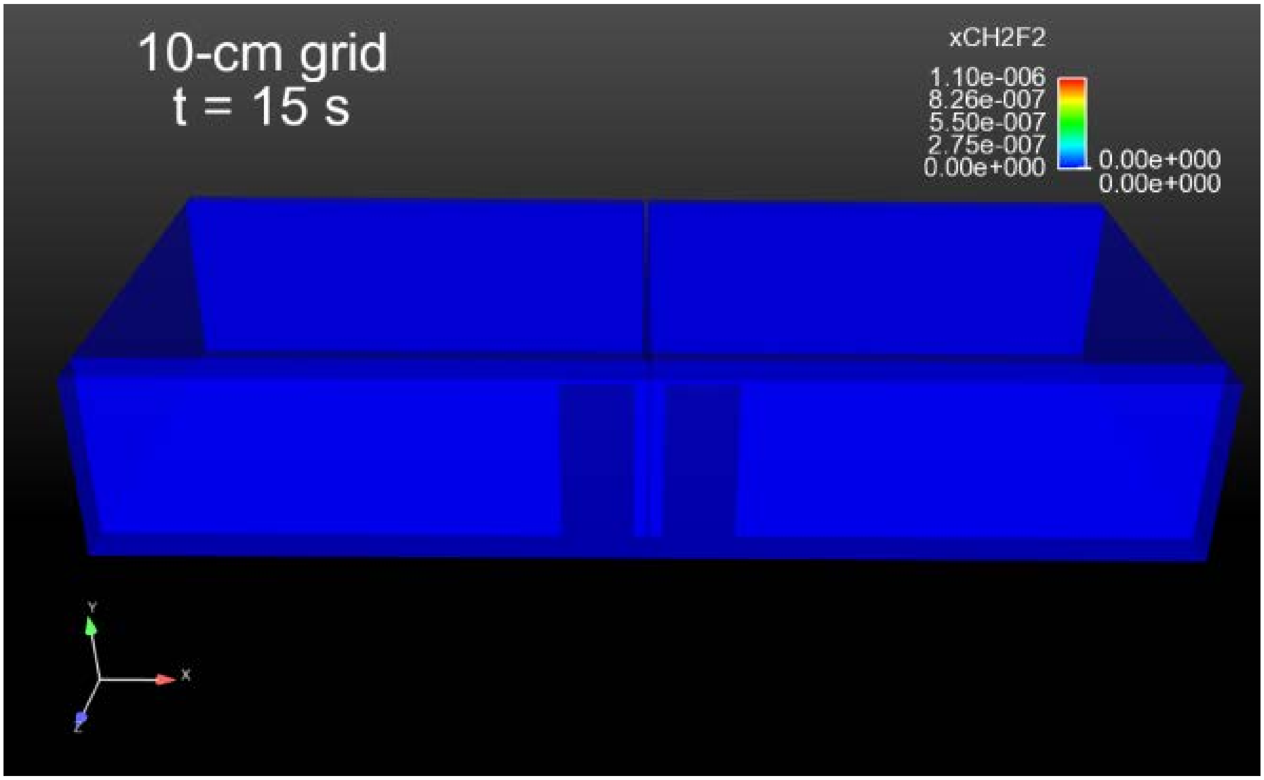
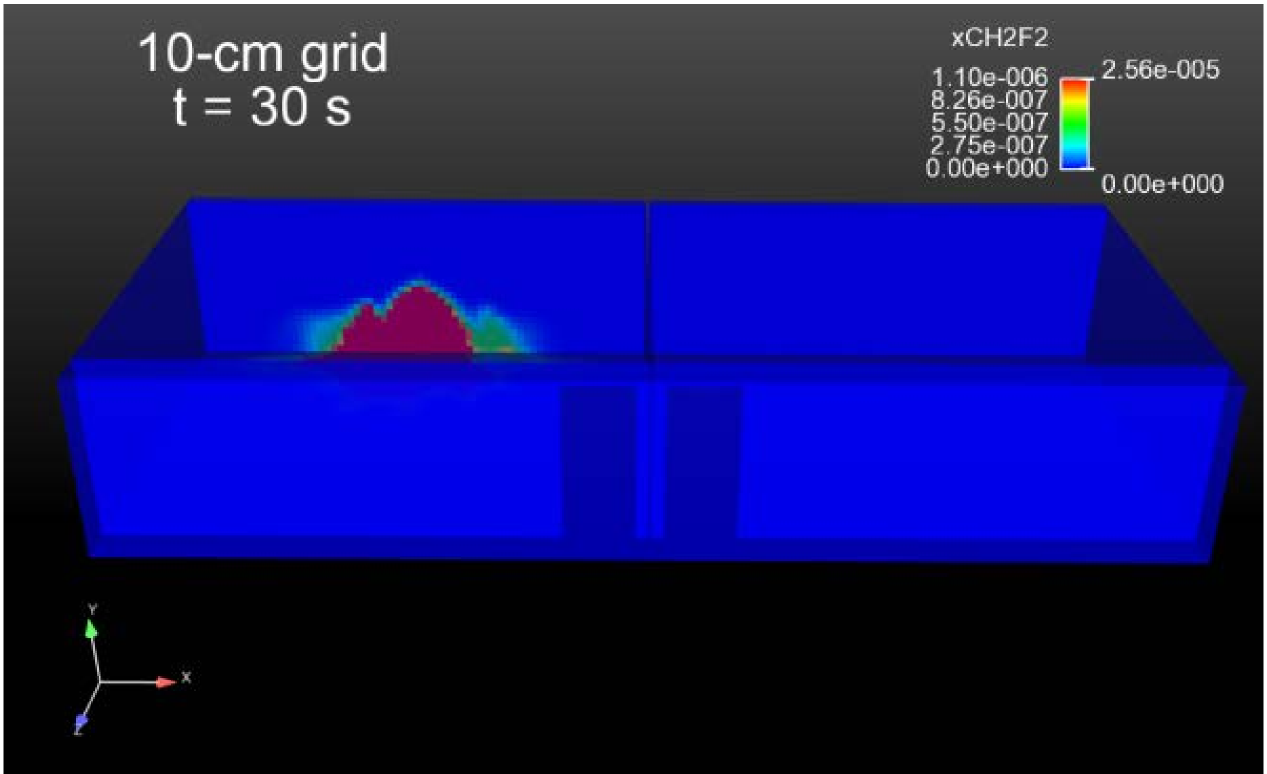


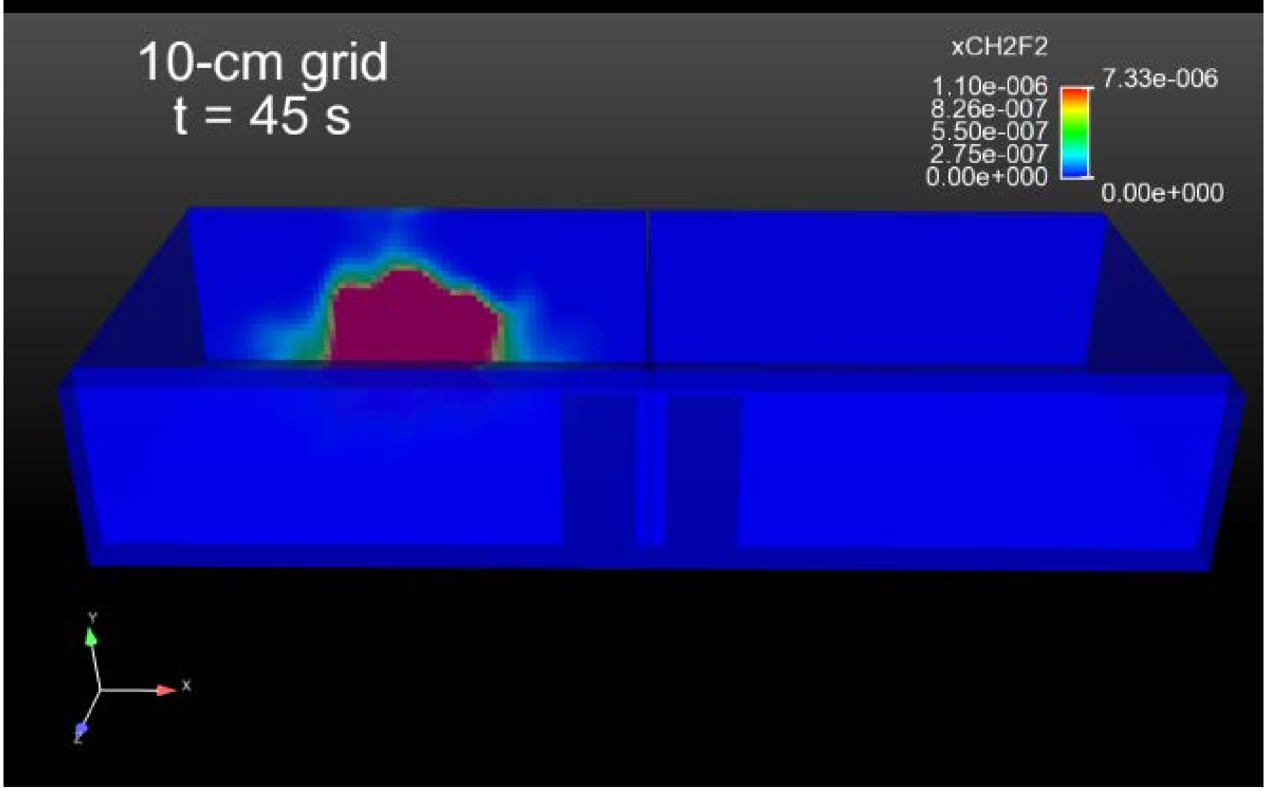
Figure 29. Contours of R-32 volume fraction in the ceiling duct at 100s, 240s, 244s, and 256s

Mass flow rate and concentration data at the outlets from the duct simulation were used to provide boundary conditions for the room simulations. Note that by doing so we essentially forced the duct simulation solution onto the room simulation. The dynamics, momentum, and mass of leaked refrigerant within the duct system were assumed to be dominant factors with the mostly quiescent, constant pressure conditions in the room having little impact on the air/refrigerant mixture leaving the duct outlets (other than the ambient pressure in the room which was applied as a boundary condition at the duct vents). This is especially true for Case 8 with system fan on forcing flow out the vents. A potential exception to this would be the composition of "makeup air" drawn into the duct (e.g. Case 2, ceiling ducts). In that case, the duct was dumping refrigerant into the hallway through the return air vent while the makeup air was drawn in through the supply vents in the rooms where refrigerant concentration remained low to negligible during the simulation (Figure 29 and 34). So, the assumption in the duct simulations that the makeup "air" was all air (with no significant refrigerant backflow) was confirmed by the room simulations.

Contour plots of predicted R-32 volume fraction inside the residential space for case 3 (underfloor ducts, fast leak, R-32) is presented in Figure 30 at different times after the start of the leak event. As expected, given that only 19g of refrigerant entered the room, the contour plots show that the refrigerant volume fraction inside each room is extremely small (maximum of 0.00256%) and isolated to the space above the floor supply registers. For the standard leak cases (1 and 4-6), no measurable amount of refrigerant entered the rooms, with all refrigerant remaining in the ducts because the low leak momentum was insufficient to overcome gravitational forces.




10-cm grid
t = 30 s
xCH2F2
1.10e-006
8.26e-007
5.50e-007
2.75e-007
0.00e+000
2.56e-005
0.00e+000
Y
X
Z


10-cm grid
t = 45 s
xCH2F2
1.10e-006
8.26e-007
5.50e-007
2.75e-007
0.00e+000
7.33e-006
0.00e+000
Y
X
Z

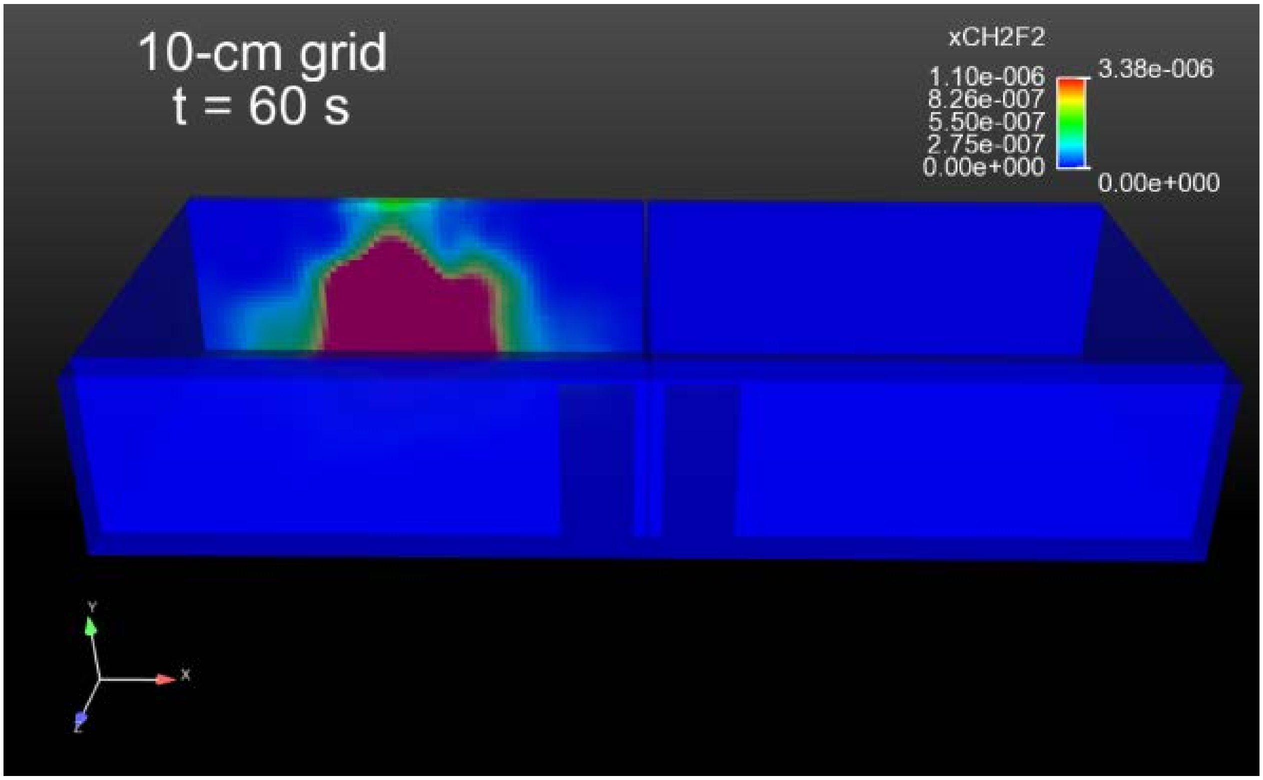


Figure 30. Contours of R-32 volume fraction inside the rooms for case 3 at 15s, 30s, 45s, and 60s

Results for the room simulation for Case 8 (with floor vents, fast leak time, and the AC indoor fan on) are illustrated in Figures 31 and 32. Figure 31 shows a room schematic with locations of three concentration monitoring points above the supply registers in each room at elevations of 0.3m (points 1 &4). 0.9 m (points 2&5), and 1.8m (points 3&6). Figure 32 provides contour plots of refrigerant concentration at six time points in the simulation. R-32 begins entering the room closest to the leak within the first few seconds, reaching ~2.5% concentration near the floor. By the 10s-point refrigerant is entering both rooms and reaches a maximum concentration near point 1 of ~5.4% (~38% of R-32 LFL, 14.4%) at the 20s-point just after the leak terminated. By the 22s-point, concentration had dropped to ~5.1% and reached ~1% at the 60s point. By the end of the simulation, fan had dispersed the refrigerant evenly throughout the room with a maximum of just under 1% near the duct outlets.

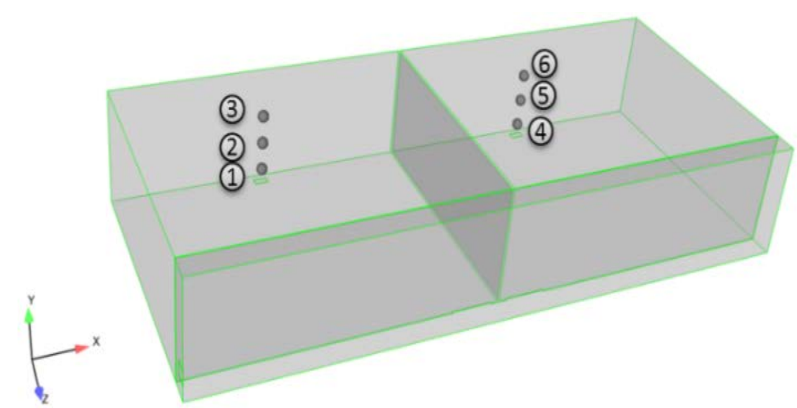
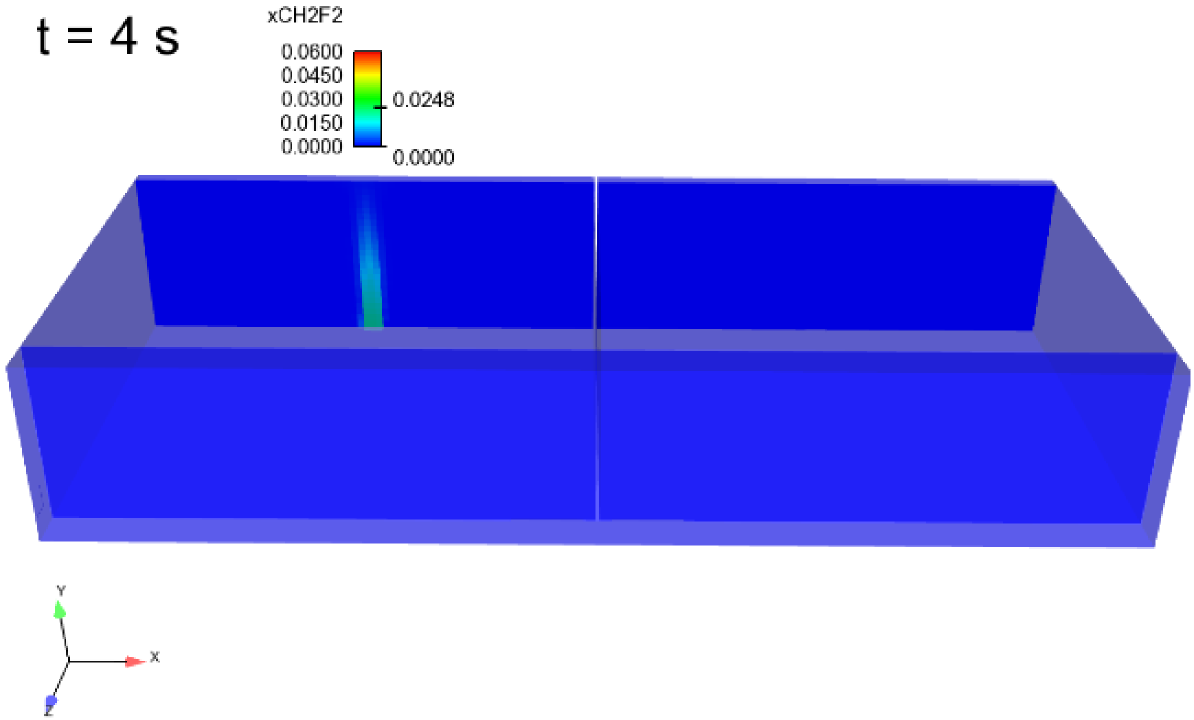


Figure 31. Half house schematic showing monitoring points (left) and R-32 concentrations vs. time at each point for Case 8 (right)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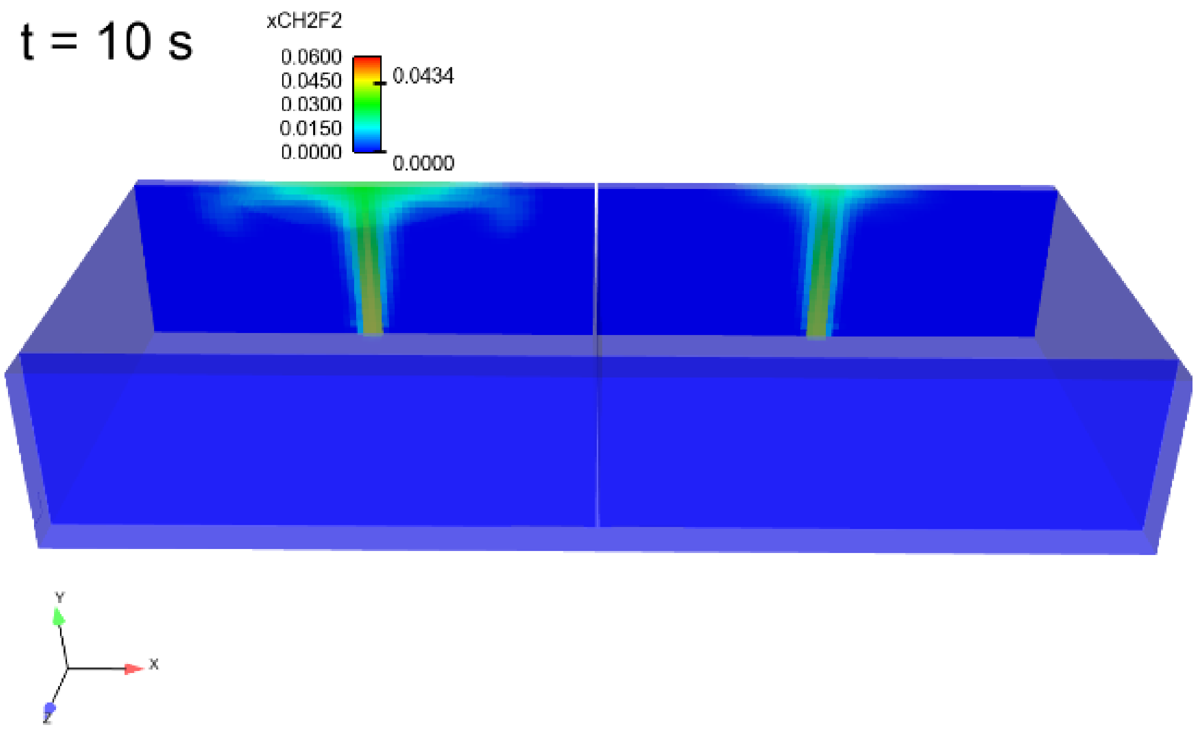
0.0450
0.0300
0.0150
0.0000
0.0248
0.0000
Y
X
Z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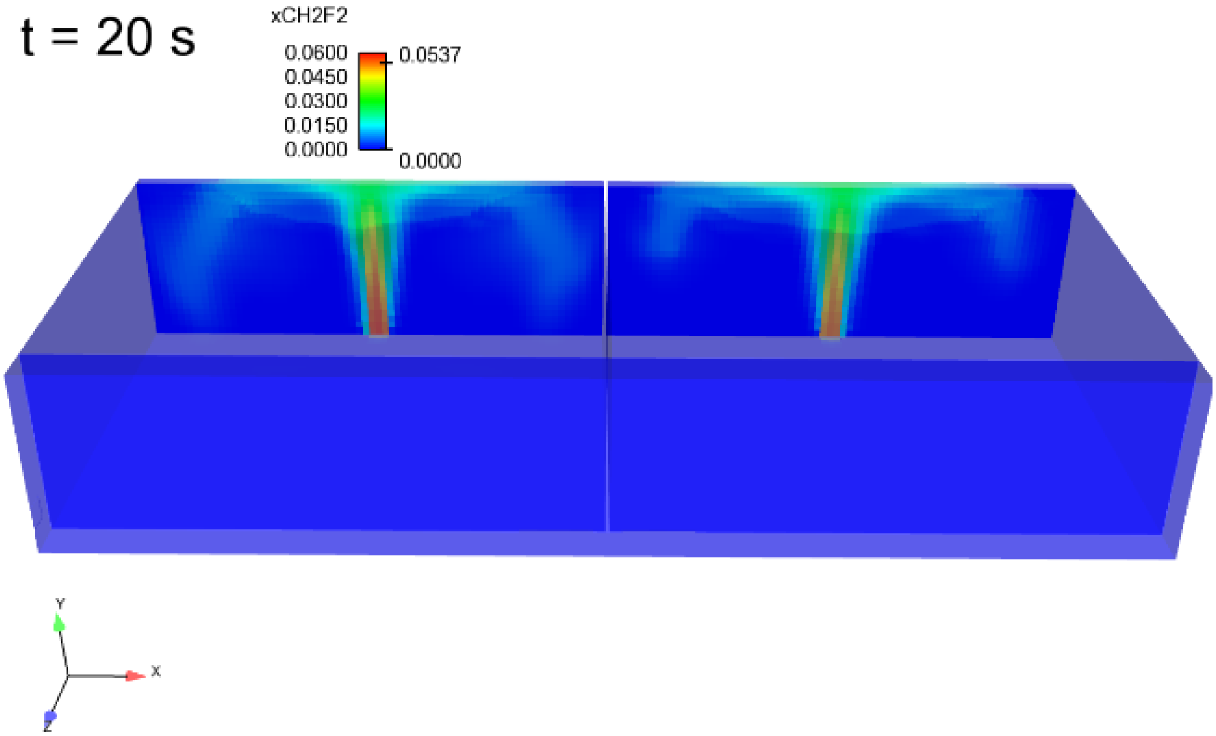
xCH2F2
0.0600
0.0450
0.0300
0.0150
0.0000
0.0434
0.0000
Y
X
Z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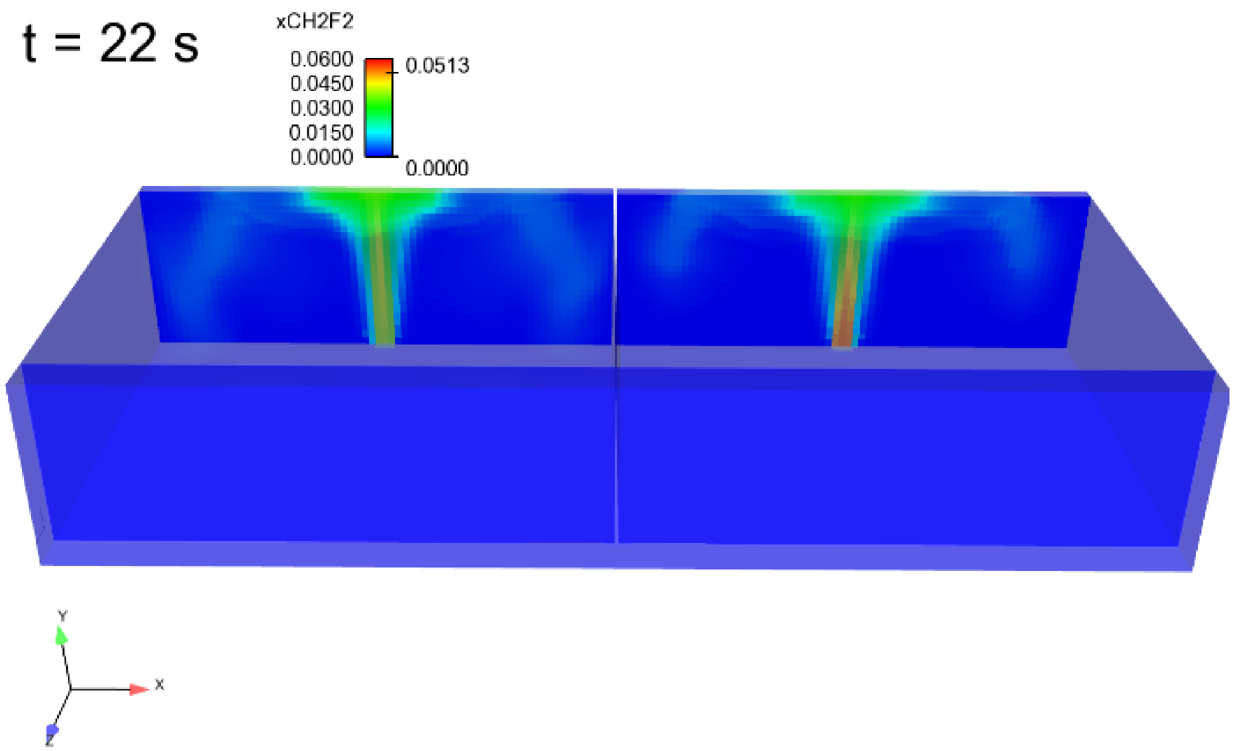
0.0450
0.0300
0.0150
0.0000
0.0537
0.0000
Y
X
Z


t = 22 s
xCH2F2
0.0600
0.0450
0.0300
0.0150
0.0000
0.0513
0.0000
Y
X
Z

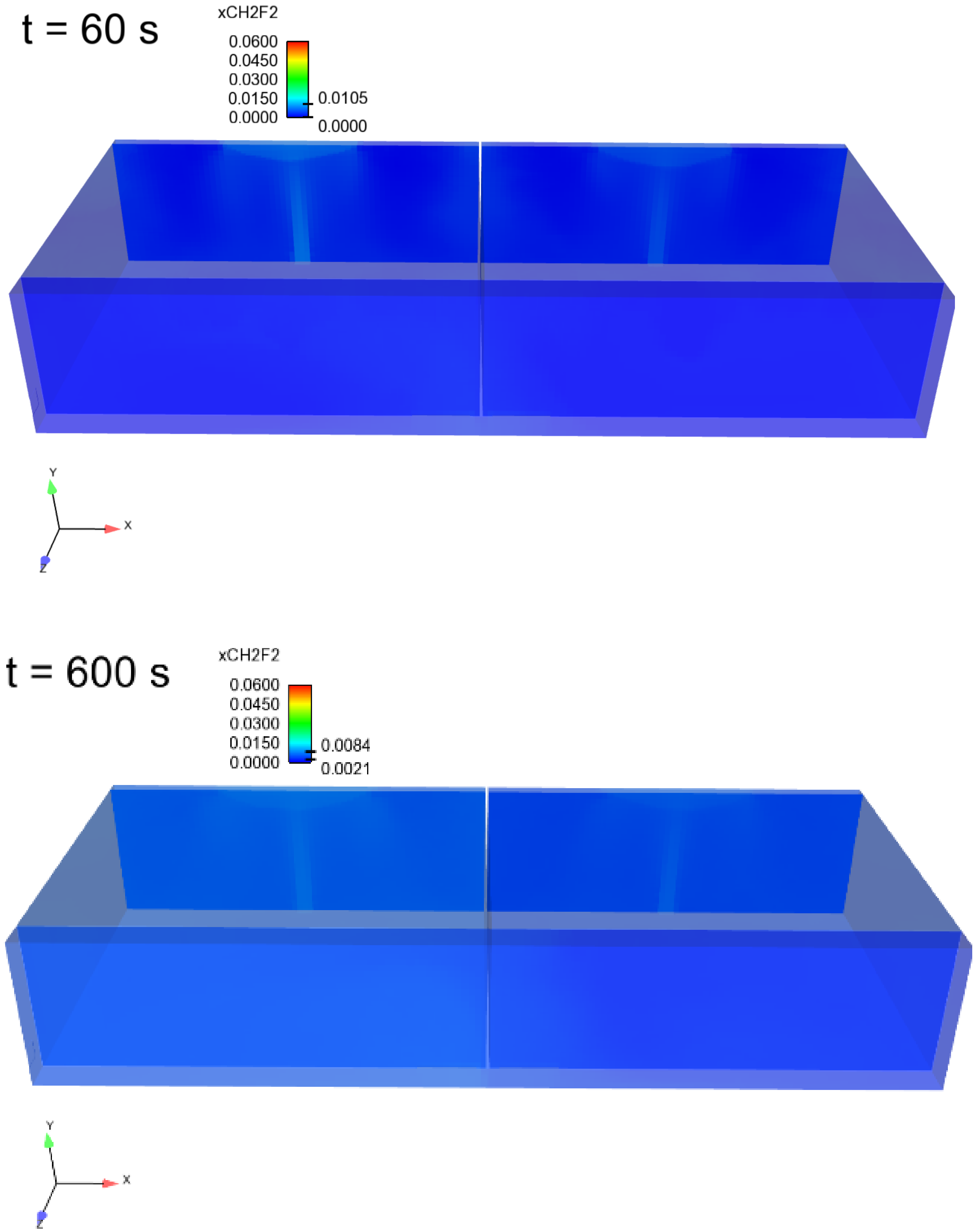


Figure 32. Case 8 refrigerant concentration contour plot at 4s, 10s, 20s, 22s, 60s, and 600s after leak start

Results for Case 2 (with attic supply air ducts) are illustrated in Figures 33 and 34 below. Figure 33 shows the mass flow rate of refrigerant/air mixture (in kg/s) at the two ceiling supply registers, outlets 1 and 2, and at the return register near the end of the leak event (240s point in simulation). Just before the leak ends, refrigerant/air mixture is seen flowing out of the supply registers at a little more than 0.1 kg/s each, while an equal amount of air flow is seen entering the return register (simulations assume no leakage from ducts to surrounding ambient air). After the leak ends, the flow reverses and the remaining R-32 flows out the return register (mixed with air) due to gravitational forces while make-up room air flows into the duct through the supply outlets. Figure 34 shows contour plots of the two rooms showing refrigerant concentration just below the supply registers for the period near the leak cessation and at the 10-min point (lower right plot). Just before the leak ends, the R-32 concentration maximum is ~3.3% or about 23% of the LFL concentration of 14.4%. Just after the leak ends (241s plot) room air begins to flow into the supply registers while R-32/air mixture flows into the hallway through the return grille. At 244s, the R-32 concentration near the return grille reaches a maximum of ~2.9% (~20% of LFL concentration). At the 10-min point all the refrigerant is relatively evenly dispersed throughout the space at ~0.4% concentration.

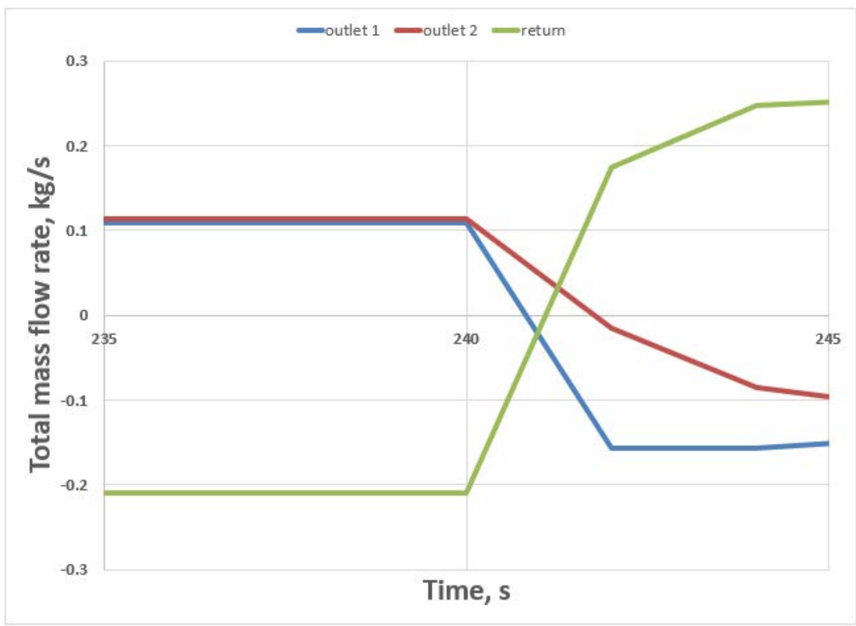
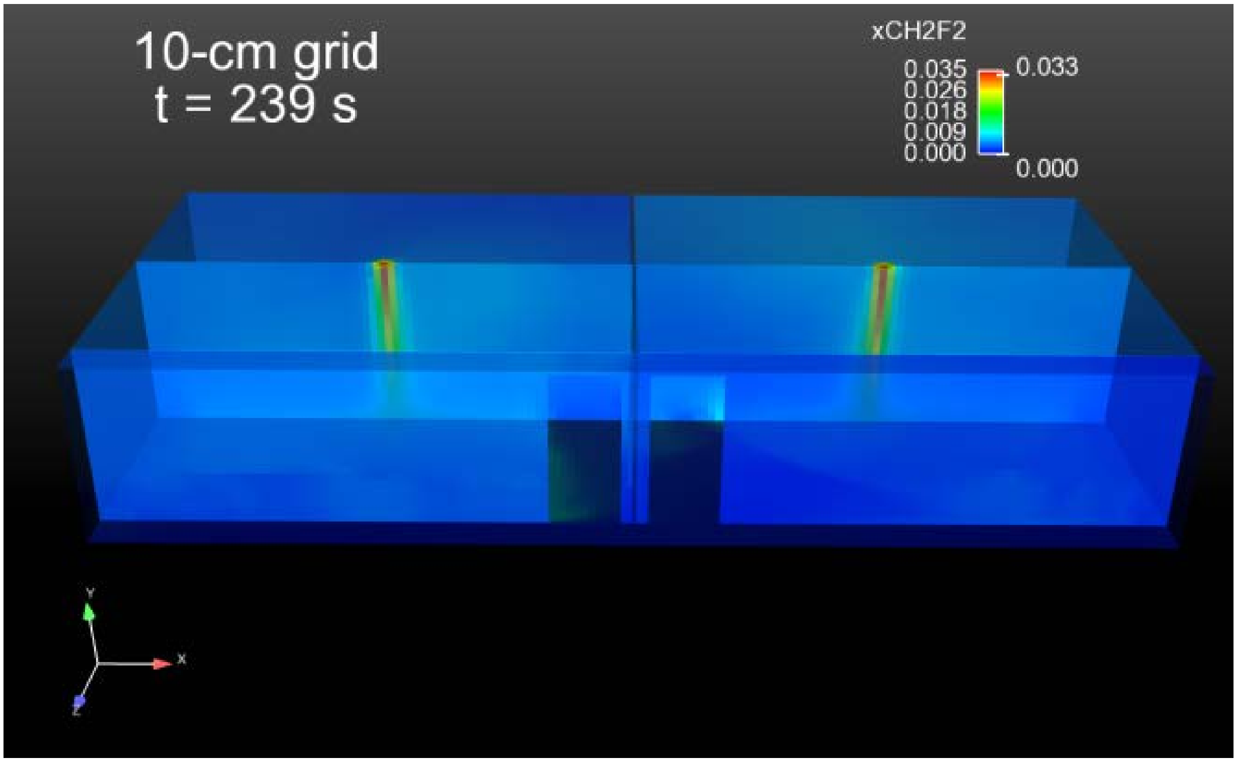
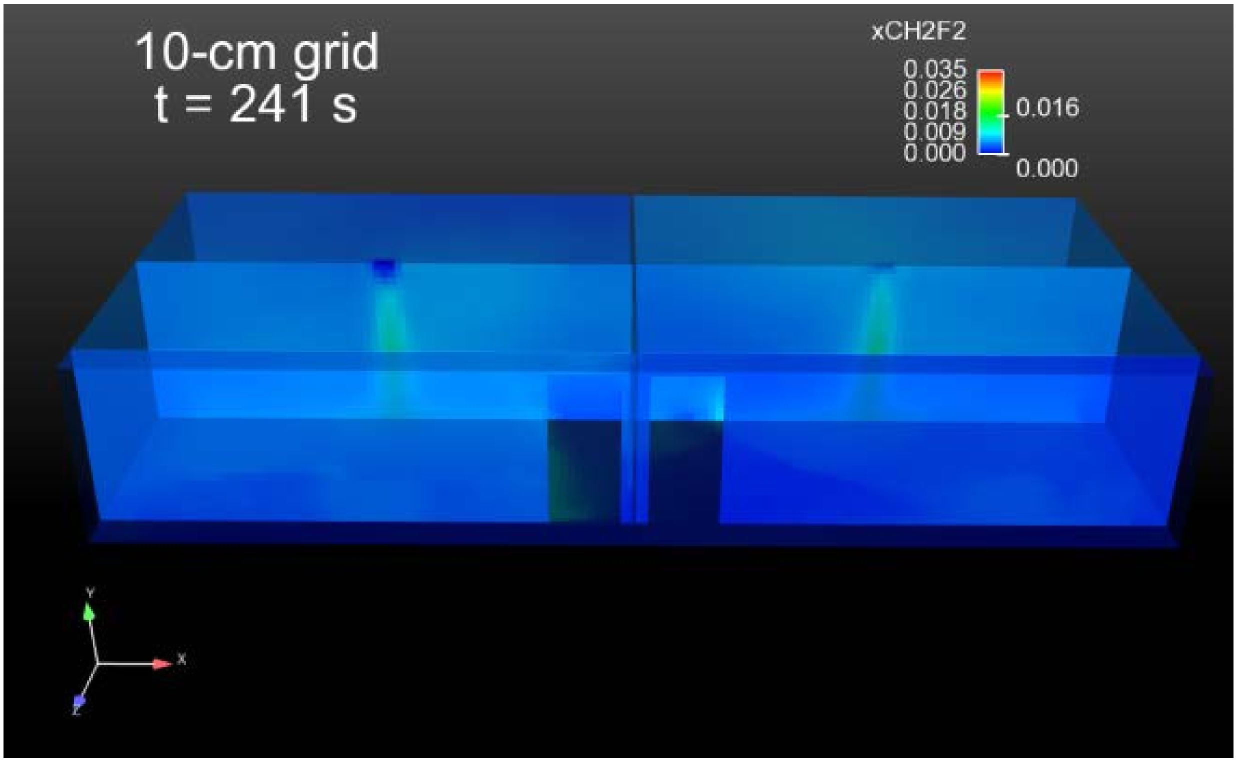


Figure 33. R-32/air mass flow at supply and return registers for Case 2 just before and after leak ends


10-cm grid
t = 239 s
xCH2F2
0.035
0.026
0.018
0.009
0.000
0.033
0.000


10-cm grid
t = 241 s
xCH2F2
0.035
0.026
0.018
0.009
0.000
0.016
0.000

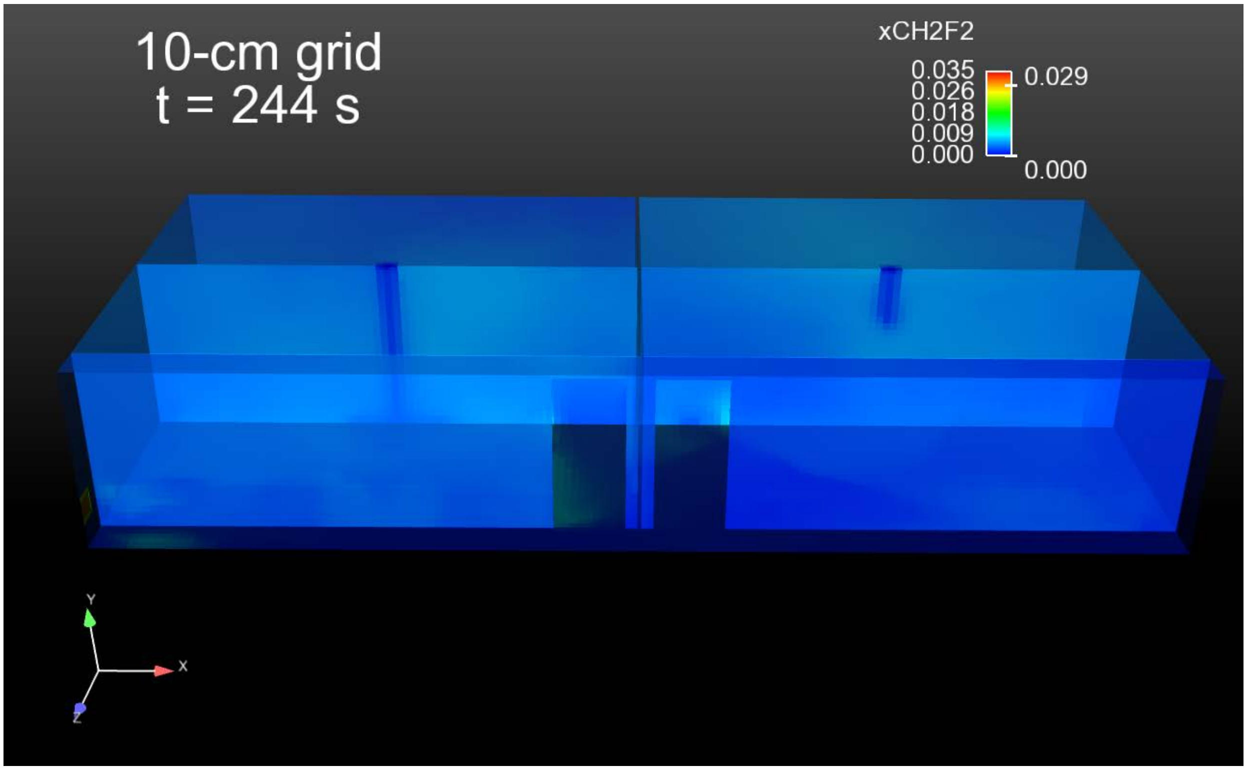


Figure 34. Contour plots of R-32 concentration in rooms just before (239s) and just after (241s and 244s) end of leak event, and at simulation end (600s)

4.4 SIMULATION OF SINGLE ROOM WITH SMALL RAC

4.4.1 Case setup

The third group of simulations was for a leak from Room Air Conditioner (RAC) with R-32 charge of 918 g. This charge amount was recommended by AHAM as being the anticipated m_1 ($m_1 = 3m^3$ x LFL) charge level in the UL 60355-2-40 update [24]. Table 13 shows the four cases simulated for different release heights and leak rates. The room design and dimensions are identical to those shown in Figure 2.

Table 13. Simulation parameters for single room with small RAC

Case #	Release height [m]	Leak rate [g/min]
1	1.8	100
2	1.8	200
3	1.8	300
4	0.6	100

4.4.2 Results

The % volume fraction of R-32 inside the room is monitored at six different points (see Table 8 for monitor point locations). Figures 35 - 38 present the volume fraction at each point as function of time for the four simulated cases. For case 1 which represents the slowest leak, the maximum volume fraction was around 4% (~28% of the R-32 LFL concentration of 14.4%) at monitoring points 1 and 4 (0.3 m elevation) at the end of the leak time as seen in Figure 35. The volume fraction gradually increased at all monitoring points (except at the first few seconds) due to the slow leak rate (550.8 seconds to leak the total charge). For cases 2 and 3, the maximum volume fraction was around 9% and 8 % (about 63% and 56% of R-32 LFL) respectively at point 3 (1.5 m elevation point closest to leak location) as seen in Figure 36 and Figure 37. For both cases, it is observed that the volume fraction tends to gradually increase while the leak is occurring, then begins decreasing. Case 4 presents a leak from a 0.6 m height source. As seen in Figure 38, the volume concentration at the lowest monitoring points (i.e. 1 and 4) show a value of ~7.3% (~51% of R-32 LFL). This value is almost double the volume fraction for case 1 for the same leakage rate. The difference is attributed to the lower leakage location which affects the refrigerant dispersion inside the room. In none of the simulated cases did the refrigerant volume fraction at any of the room monitoring points exceed the LFL concentration of R-32 (14.4%).

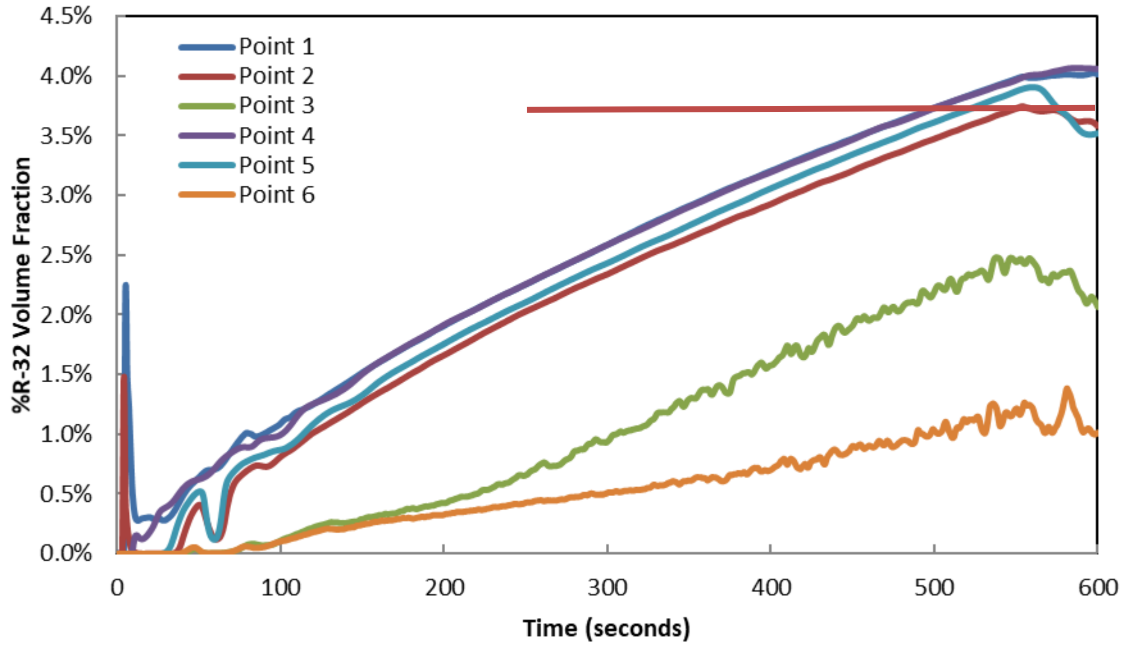


Figure 35. % volume fraction of R-32 at six monitoring points for case 1 [NOTE: the solid horizontal line illustrates a concentration of 3.6% (25% of the R-32 LFL)]

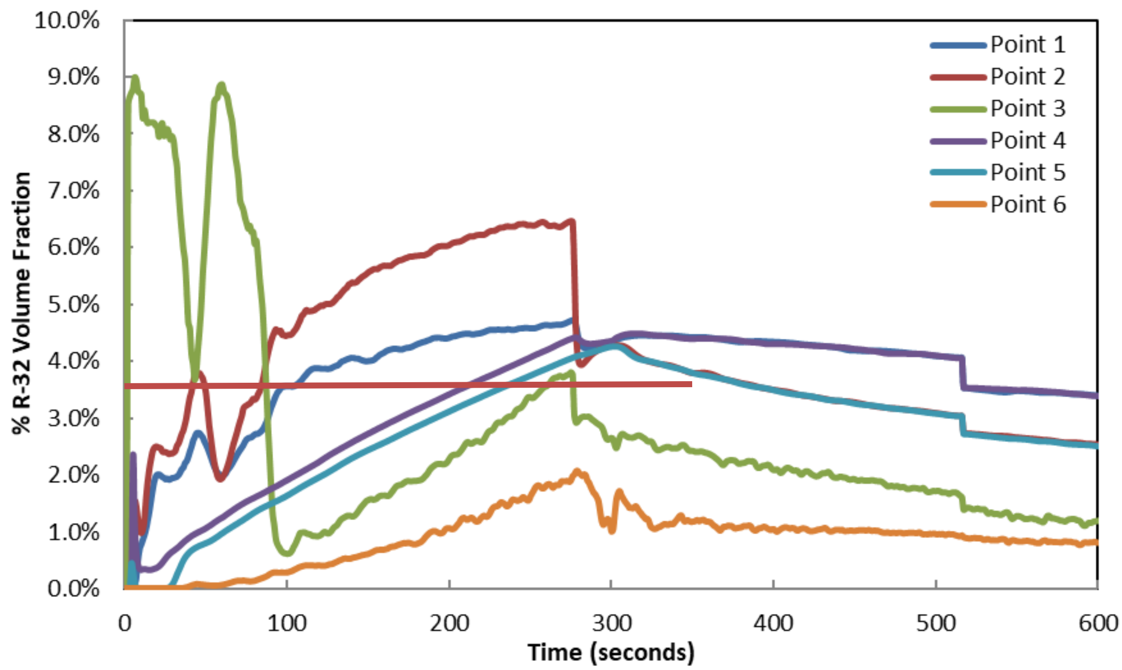


Figure 36. % volume fraction of R-32 at six monitoring points for case 2 [NOTE: the solid horizontal line illustrates a concentration of 3.6% (25% of the R-32 LFL)]

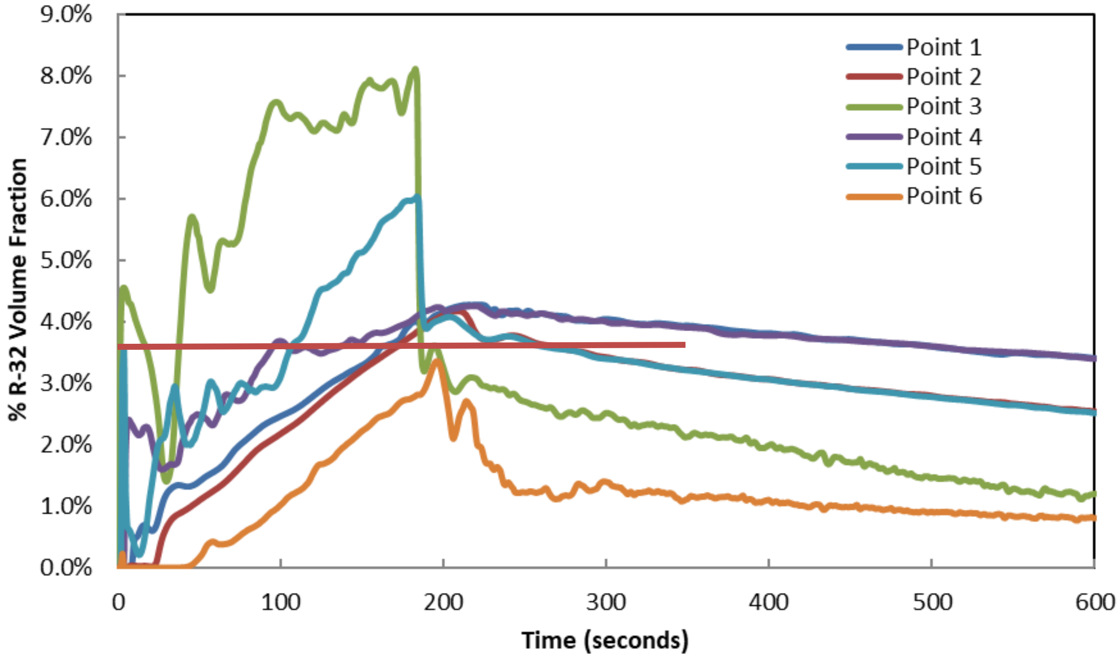


Figure 37. % volume fraction of R-32 at six monitoring points for case 3 [NOTE: the solid horizontal line illustrates a concentration of 3.6% (25% of the R-32 LFL)]

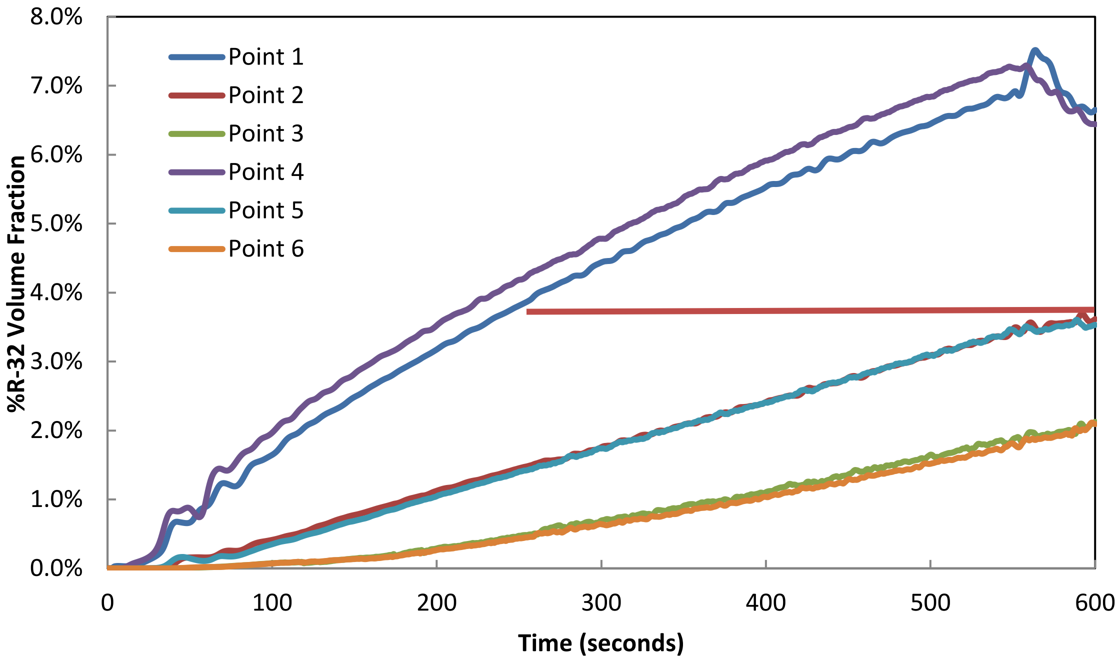


Figure 38. % volume fraction of R-32 at six monitoring points for case 4 [NOTE: the solid horizontal line illustrates a concentration of 3.6% (25% of the R-32 LFL)]

To further characterize the flammability risk for the simulated cases, the flammable volume (which is defined as the volume where R-32 volume fraction is between LFL and UFL) was integrated in space and presented in Figure 39. For cases 1-3 (all for 1.8 m release height), the flammable volume maximum value is proportional to the leaked refrigerant mass flow rate, while the residence time of the flammable volume is inversely proportional to the leak flow rate. The maximum flammable volume is seen for case 4 (~3 liters) while the minimum flammable volume is seen for case 1 (~0.9 liters). One can see that the leak source height plays a significant role in the flammable volume existence inside the room. For case 4, the leaked refrigerant is released at a lower elevation which concentrates the refrigerant dispersion nearer the floor, increasing its volume concentration and accordingly the flammable volume. After the leak stops, the flammable volume dissipates as the refrigerant continues to mix with the room air. The flammable volume for all cases was observed close to the leak source at the wall.

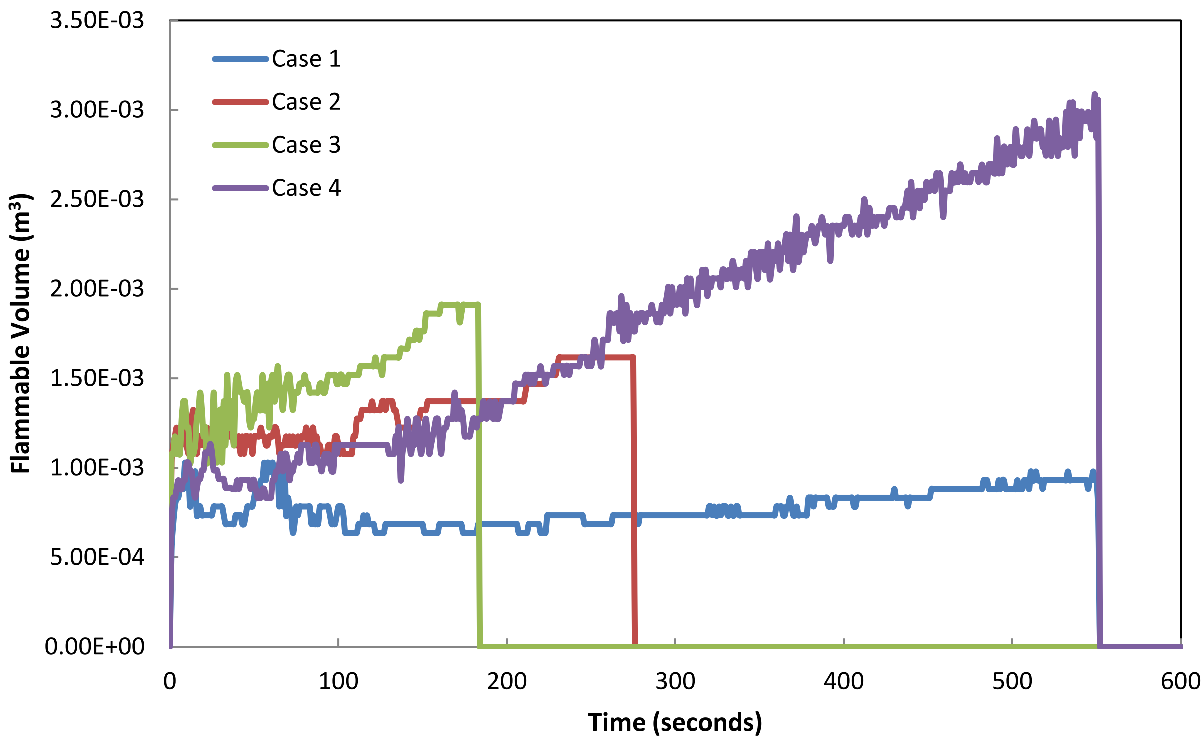


Figure 39. Total flammable volume inside half the room

4.5 REDUCED ORDER MODEL (ROM) SIMULATIONS & DEVELOPMENT

The final stage of this project involves completing a series of CFD single-room simulations to support formulation of a reduced order model (ROM). The goal is to develop a relatively simple approach that industry and safety standards developers can use to estimate safe refrigerant charge limits for a range of refrigerant release parameters.

The ROM intention is to develop a correlation based on the parameter ranges given in Table 14, below, to estimate refrigerant concentration profiles inside a single room in the case of a leak from a wall mounted unit or any similar point source leak. Taking this information together with flammability characteristics of a given refrigerant, it should be possible to estimate maximum safe charge limits for that refrigerant. The room will have the same aspect ratio (3:4) and height (8 ft) as that shown in Figure 2 above and three different floor areas, as shown in Figure 40. The leak locations, supply and return air grills are shown in Figure 41. A range of refrigerant molecular weights from 44 to 114 g/mol are used to cover R-290, R-32, R-452B, R-454B, and R-1234. A refrigerant charge range representing $0.75*m_{max}$, m_{max} and $1.5*m_{max}$ for each of the refrigerants will be used (as before, the maximum refrigerant charge, m_{max}, is calculated according to formulas in IEC 60335-2-40 [4] for a given refrigerant). Cases will be run for both unit blower off and on, with separate ROMs expected. A total of about 600-700 individual CFD simulations will be executed for the ROM development. The general setup for all the CFD cases is described in Table 7. The CONVERGE adaptive mesh refinement (AMR) tool is being used on these runs to allow use of a coarser base grid which is only refined in areas where high sub-grid property gradients are predicted. Specifically, a cubic base grid of 0.1 m will be used to model the three room sizes resulting in base mesh sizes of approximately 14,000, 30,000, and 54,000 cells. AMR subgrid tolerances are set to 1 m/s for velocity and 0.5% for mass fraction of refrigerant with a minimum grid size of 0.0125 m. If the velocity or refrigerant concentration are predicted to vary across a cell by more than the specified tolerance, CONVERGE will automatically sub-divide that cell into smaller cells until either the subgrid tolerances are no longer exceeded or the minimum cell size is reached. This approach provides a more accurate solution than the coarse mesh alone with less computational requirements than a refined mesh across the full domain.

CFD simulations for ROM development are underway and results will be presented in the second volume of the project report.

Table 14. Reduced Order Model (ROM) parameters

Parameter #	Parameter	Parameter type	Range
1	Refrigerant type	Continuous	Molecular weight range ~ 44 - 114 g/mol
2	Leak rate	Continuous	3 levels suggested (range 3.75 to 45 kg/min)
3	Room size (volume)	Continuous	Room footprints: 9’ × 12’ base, 12’ × 18’, 18’ × 24’.
4	Leak release height	Continuous	0 m (floor), 0.61 m, 1.22m, 1.83 m, 2.44 m (ceiling)
5	Charge amount	Continuous	0.1 to 15 kg
6	Ventilation	Continuous	~ 0 - 576 cfm
7	Room openings	Continuous	Variable door openings (closed with open floor gap, half-open or door louver, full open)
8	Air circulation	Discrete	Unit blower on or off, 500 cfm

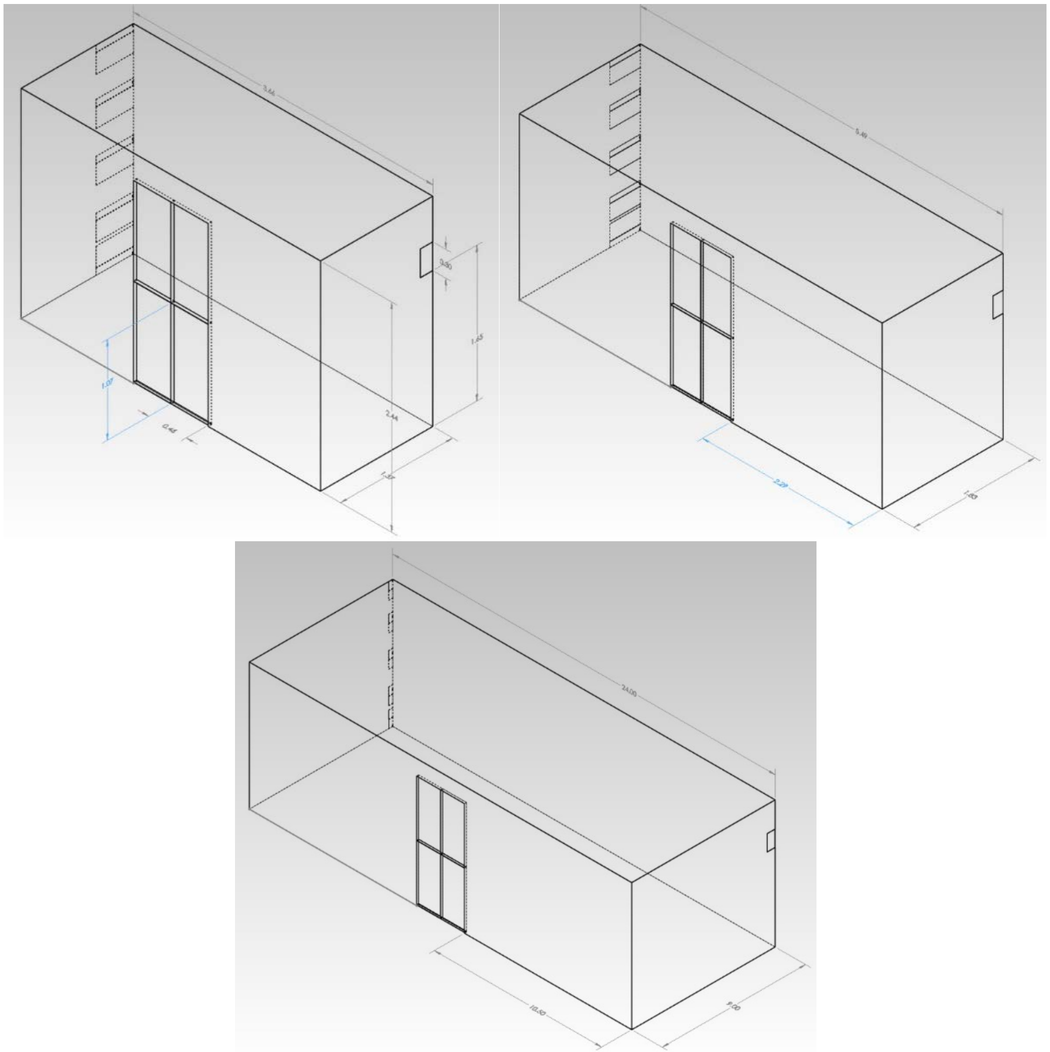


Figure 40. Three single room designs for ROM simulations (dimensions in meters)

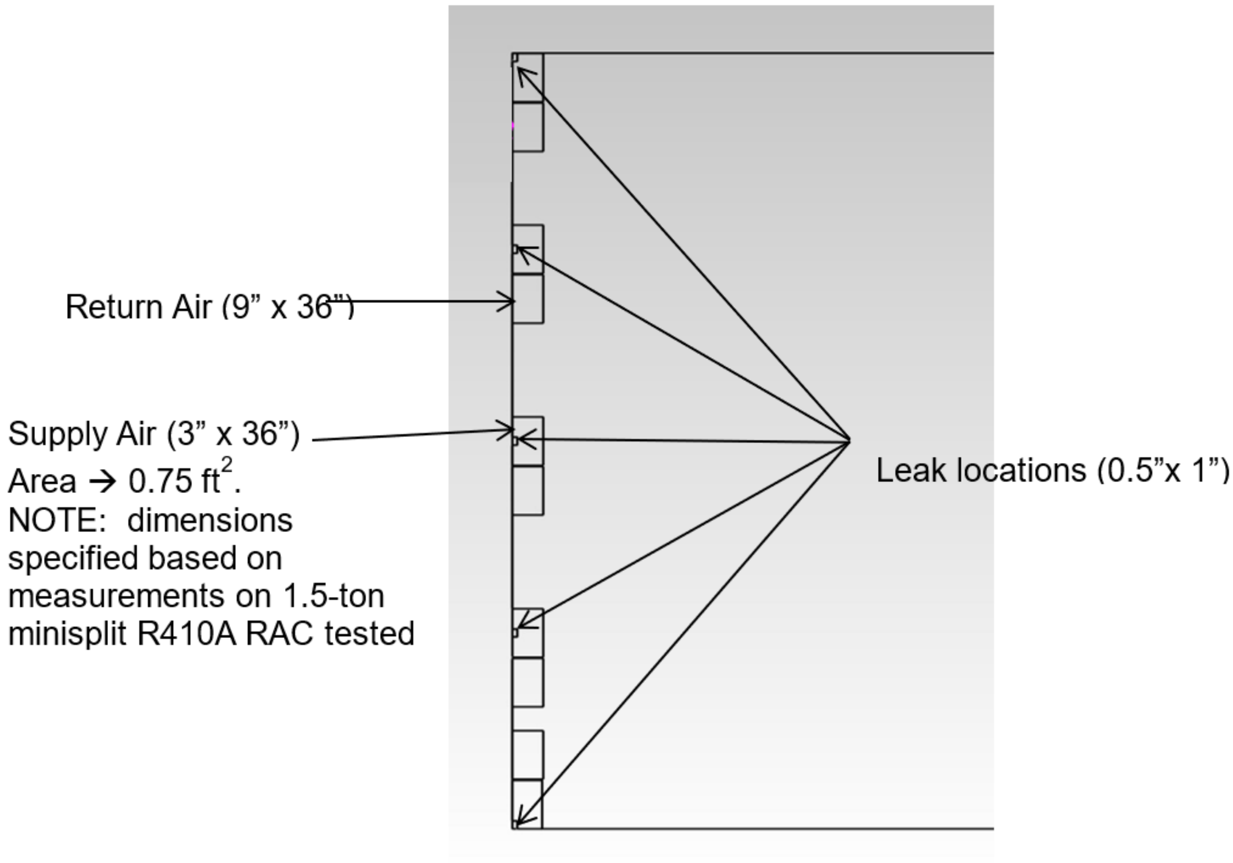


Figure 41. Locations of leak release, supply and return air diffusers

5. CONCLUSIONS

This report is the first of two planned to provide an overall summary of the approach and tasks of the ORNL Flammable Refrigerant Charge Limits Estimation project. In this volume, summaries of the initial stakeholders' workshop, prior literature and research survey, and the computational fluid dynamics (CFD) modeling approach, calibration and validation, and testing are presented. Simulations of a 4-room single-family home and duct system are presented along with summary results and concluding observations. Several refrigerant leak case simulations and results for small room ACs are discussed as well.

This volume also provides a description of the approach for development of reduced order models (ROM) for estimation of safe charge limits based on a computational fluid dynamics (CFD) parametric study. Fuller details of the ROM development are to be provided in the second project report.

5.1 WORKSHOP

ORNL held a workshop on October 24th of 2016 to solicit critical input from stakeholders in industry and other organizations to help guide the project and achieve results most useful to the US HVAC&R and Appliances community. ASHRAE hosted the workshop at its Atlanta Headquarters Offices. The workshop engaged the stakeholders in discussions related directly to the project as well as other relevant issues related to the wider adoption of flammable refrigerant by the market. The workshop program began with an initial presentation followed by four breakout sessions for detailed discussion of relevant topics.

- The first breakout session focused on the R&D gaps in the field of flammable refrigerant application.
- The second breakout session focused on the scope of the standards and how comprehensive they are.
- The third breakout session focused on the most important factors to consider in the CFD analyses to be conducted.
- The fourth breakout session focused on the practical aspects that should be considered in CFD analysis.

After the breakout sessions, a final session was held to discuss and prioritize the most relevant case studies to be pursued for further analysis. Tables 15-19 below summarize priority ideas/suggestions arising from the four breakouts and the final session.

Table 15. Ideas and suggestions from breakout session 1a (What are the relevant R&D gaps?)

Idea/suggestion	Votes
Evaluating the severity of refrigerant combustion event	17
Characterization and probability of leaks	16
Minimum worst-case scenario leak rate for each type of equipment	14
Available ignition energy of common electric components	11
Necessity of validating the CFD results	11

Table 16. Ideas and suggestions from breakout session 1b (Do we have enough information in the safety standard?)

Idea/suggestion	Votes
Impact of certification requirements of technicians	18
Developing training modules and standards for servicing flammable refrigerants equipment	17
Impact of UL, ASHRAE and AHRI standards updates timeline vs building code update timeline	11
Split system exclusion from hydrocarbon use	10

Table 17. Ideas and Suggestions from breakout session 2a (What are the most important factors to consider in the CFD analyses phase of the project?)

Idea/suggestion	Votes
Release locations	12
Boundary conditions	12
Variable vs. constant leak rate	10

Table 18. Ideas and Suggestions from breakout session 2b (What are the practical issues that we need to study?)

Idea/suggestion	Votes
Leak rate assumptions	13
Effectiveness of detection and circulation (ducted and ductless)	11
Utility closet	10

Table 19. Ideas and Suggestions from Case Studies Session

Idea/suggestion	Votes
Room that meets minimum floor area requirements for m_2	13
Leak profiles in various applications of RTU, mini split and VRF units	10
Validate the underlying premise of the standard for m_1, m_2 and m_3	5
Residential split heat pump air handler unit in utility closet	2

5.2 LITERATURE REVIEW

International standards and refrigerant safety classification standards from ASHRAE, ISO, and IEC provide information about permissible locations for systems employing flammable refrigerants, corresponding maximum quantities of refrigerant charge, construction requirements for the mechanical systems and external features associated with installation, such as ventilation and detection. The standard which is most relevant to the current work is IEC 60335-2-40. In view of the fact that the HVAC&R industry is becoming increasingly global in nature, developers of safety and other standards (in North America and the rest of the world) are engaged in an effort to align their respective requirements to facilitate their application worldwide. The US Underwriters Laboratories (UL) embodiment of IEC 60335-2-40 is called UL 60335-2-40. Below is a list of the main issues impacting flammable refrigerant usage in IEC 60335-2-40:

1. Flammable refrigerant charge limits and equations were initially developed for A3 and A2 refrigerants. Current proposals to allow higher charge limits for A2L refrigerants should be verified for safe use.

2. The most conservative conditions were used at the time of development of the standard: low leak velocity, fixed 4 min leak rate, downward leak direction, tight room, no ventilation, no oil presence, no air flow. These conditions may prove to be overly restrictive for newer A2L refrigerants which have relatively high minimum ignition energy and low burning velocity, especially if sufficient mitigation is present.

3. The effect of the presence/absence of obstacles on refrigeration dispersion is also not well understood.

5.2.1 Experimental and numerical studies

The determination of appropriate charge limits depends on, among other things, information on both the spatial and temporal variation of the flammable refrigerant concentration. Many experimental and numerical studies were found in the literature for both A2L and A3 refrigerant leaks. For most studies reviewed, it was determined that aside from flammable refrigerant concentration and dispersion data, there was no clear connection to the maximum charge limits prescribed by the standards. A summary of the studies is depicted in Figure 42 illustrating the relationship between flammable refrigerant charge limits (according to standards), actual charge, maximum concentration and LFL.

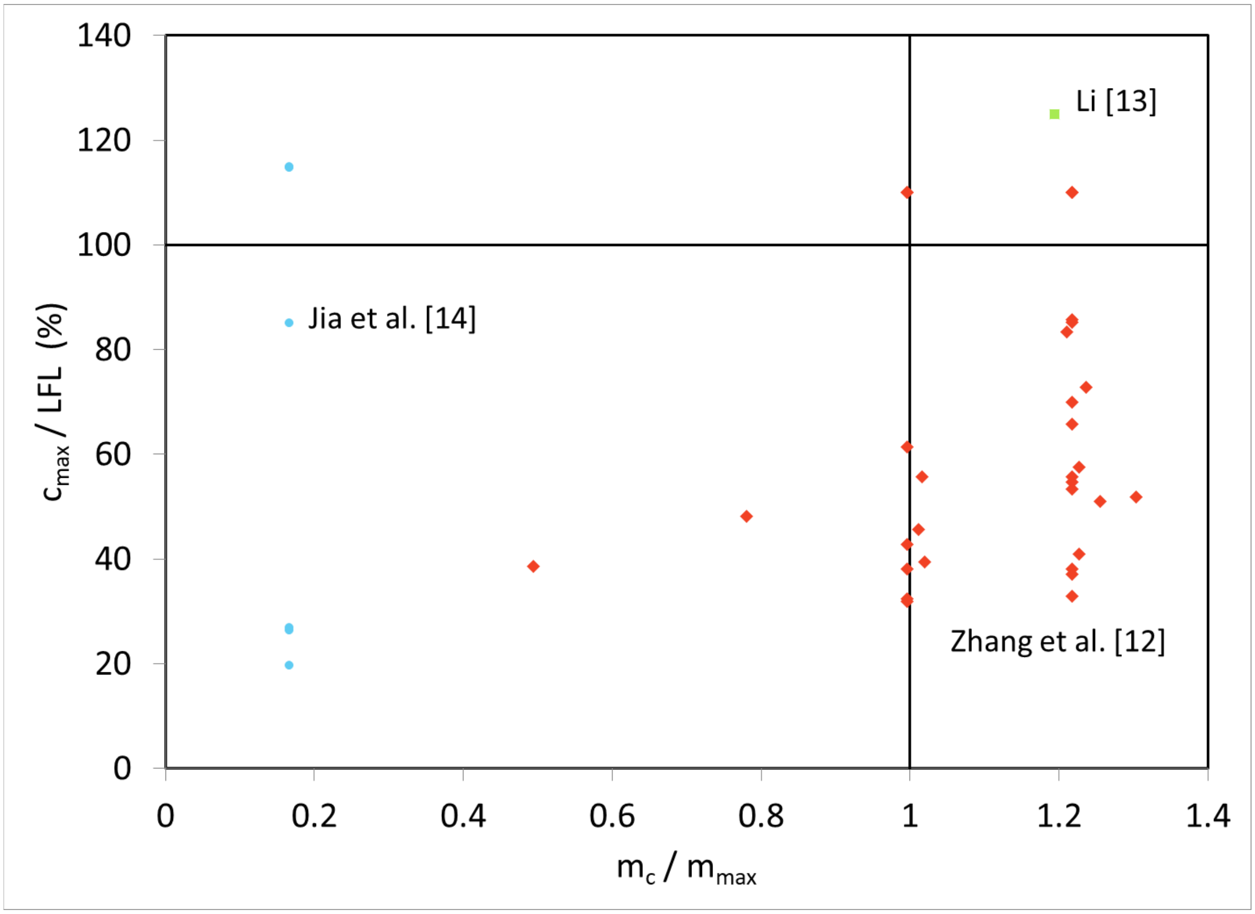


Figure 42. Pictorial summary of a sample of flammable refrigerant dispersion studies

The main conclusion from the analysis and review of recent experimental and numerical studies was that the results of such studies should directly connect to the corresponding maximum charge as calculated by the pertinent standard, to determine the practical impact of the research. As seen in Figure 42, there are numerous cases where the refrigerant charge is greater than m_{max} while the maximum observed concentration was less than the LFL. There are also cases with very low refrigerant charge but with observed refrigerant concentration in excess of the LFL. The reference sources note that the maximum concentration measurements are quite dependent upon sensor location.

5.2.2 Probabilistic risk assessments of different systems

Probabilistic Risk Assessment (PRA) is a systematic methodology to evaluate risk in a system. In the context of flammable refrigerants, PRA is used to determine probability of a fire or explosion event occurring because of a leak of flammable refrigerant from equipment or appliances. PRA studies depend on fault tree analysis. The most important factor was the probability of refrigerant concentration reaching the LFL due to a leak, which was found from experimental measurement and CFD simulations of refrigerant concentration mapping.

5.2.3 International guides and resources

In addition to the published journal articles and reports concerning flammable refrigerant leaks and probability risk assessments, various international guides and other resources were also found during the literature review. These have been created in several countries by their respective governmental entities, industrial partners and academic institutions for the safe use and handling of flammable refrigerants. This report lists organizational efforts from Japan, Germany, Great Britain, and Australia.

5.3 COMPUTATIONAL FLUID DYNAMICS SIMULATIONS

The core effort in this project involved simulating various refrigerant release scenarios using computational fluid dynamics (CFD) models. Two commercial software platforms, FLUENT™ and CONVERGE 2.3.17 were used. Results were post-processed using Ensight™ 10.1. The CONVERGE geometry models were built first in SolidWorks™ then exported to CONVERGE STUDIO for CFD simulation setup. To reduce computational requirements, the cases were set up to take advantage of symmetry where possible so that only half the domain needed to be modeled. Three major categories of leak scenarios are described in this report: (1) initial simulations of a leak from wall-mounted air-conditioning (AC) unit into a single room coupled with testing for validation of the CFD models, (2) leaks from a package AC unit into a multi-room residential space, (3) leaks from a small room AC (RAC) unit into a single room.

5.3.1 Single Room with Wall-Mounted AC Unit – Initial CDF Simulation and Calibration Results

The room geometry for the analyses and calibration tests under this scenario is shown in Figures 2 and 17. Six monitor point locations were created in the model corresponding to the experimental sample locations to allow comparison of measured and predicted refrigerant concentration profiles. An initial set of simulations using this geometry were performed to develop simulation protocols and serve as proof-of-concept. R-32 was used for these initial simulations and tests. The impact of total refrigerant charge (or leak amount), leak flow rate, and leak release height as well as the presence or absence of room obstructions were investigated. A total of 12 cases were constructed to represent a baseline (based on the maximum refrigerant charge allowed per IEC 60335-2-40 and standard leak rates and conditions) and cases exploring release rate, release height, charge quantity, internal obstacle, and ventilation impacts. Table 11 describes the test cases. The leak release area was specified as a 0.305 × 0.305 m (1 × 1 ft) grate. For simplicity, the leak was modeled as a constant, mass-flow boundary condition across this area for the duration of the leak, which is the time needed for the full charge to leak at the specified rate. Based on a grid-convergence study to optimize accuracy and computational time, a uniform 3.5 cm grid was selected.

The FLUENT™ CFD simulation results showed significant level of stratification of R-32 concentration and were consistent with the results from CONVERGE. The assumption of uniform distribution of the flow across a large leak area (0.093 m^2) resulted in low-momentum flow of refrigerant entering the room and immediately cascading down the wall under the influence of gravity for all leak rates simulated.

Maximum concentration for Baseline, Case 1, was ~13%, very near the R-32 LFL concentration of 14.4% (per ANSI/ASHRAE 34-2016). Doubling the AC unit charge had a significant impact, raising the maximum concentration to more than 23%, exceeding the LFL level. Adding ventilation showed little impact on R-32 concentration near the floor. Figure 16 above illustrates total fraction of the room volume with a flammable concentration of R-32 (concentration between LFL and UFL) vs. time for several of the Cases. For the Baseline Case 1, about 2% of the room volume held a flammable concentration for about 40 s. Case 5 (slow leak) showed no flammable volume. Doubling the charge showed about 50% maximum flammable volume with or without ventilation (Cases 3, 11, and 12). With a fast leak, Case 4, there was ~20% flammable volume. Lowering the release height from 1.5 m to 0.9 m showed also a maximum flammable volume of ~20% but it dissipated more quickly (lower total charge release).

To calibrate the proposed CFD models, tests were performed to study the release of flammable refrigerants into a single room for different scenarios and operating conditions. The tests were performed at Jensen Hughes in Baltimore, MD. The refrigerant used during the tests was R-32. The tests involved variation in refrigerant charge, flow rate, release height, presence/absence of ventilation and presence/absence of obstacles. The effect of these variables on refrigerant concentration was measured and documented for comparison to CFD predictions and calibration of the models.

A total of 21 tests were conducted, covering the 12 refrigerant discharge scenarios, and data were successfully obtained on the diffusion and mixing of refrigerant R-32 when released into an enclosure. Test 1 was the baseline case for use as a comparison for evaluating the effects of variables such as the release height, refrigerant flow rate, discharge duration or total mass released, phase of the refrigerant (liquid or vapor) during the release, presence of obstructions and presence of operating ventilation. The most critical data were obtained from measurements of refrigerant concentration as a function of time and at various locations in the enclosure.

Comparing experimentally measured concentration gradients with the initial simulation results at similar conditions indicated that less charge stratification was observed than initially predicted by the models. As mentioned above, the leak was applied as a uniform mass-flow boundary condition across the return air grill in the initial simulations resulting in a low-momentum cascade of refrigerant exiting the grill and flowing to the floor producing the high concentration gradients. However, observations of the leak release during the calibration testing and shakedown testing of the release duct indicated that the refrigerant enters as a relatively high momentum plume. Therefore, several approaches were tested in CONVERGE to develop a more accurate representation of the observed leak release pattern. By simply varying the area through which the leaked refrigerant enters the room using a square grid ranging in size from 0.305 m to 0.001 m equivalent diameter. It was determined that a release grid of ~25 mm (1 inch) equivalent diameter produced the best match.

The calibrated CFD code and room profile of this scenario will be used in the final stage of the project; formulation of two ROMs (one with unit blower off and a second with the blower on). A total of about 600-700 individual CFD simulations will be executed over the parameter ranges given in Table 14 for each ROM development. These simulations are underway, and results will be presented in the second volume of the project report.

5.3.2 Multi-Room Residence with Package AC Unit

This scenario involved simulations of refrigerant releases from a 10.55 kW (3-ton) package AC unit (16 SEER, 3.175 kg (7 lb) charge) connected to duct system serving a 167.23 m^2 (1800 ft^2) 4-room residence. A total of nine cases were simulated, seven with R-32 and two with R-452B. Both floor and ceiling ducts were simulated. Two leak durations were simulated: a slow leak (4-min duration) and a catastrophic) leak representing a rupture of a 6.35 mm (¼") internal diameter pipe downstream of the evaporator coil. For this case, the leak flow rate was computed to be 0.1786 kg/s (0.393 lb/s). Table

To further improve the computational time, simulation of the refrigerant flow through the duct was conducted separately from that of the refrigerant dispersion throughout the larger space. This approach ensured adequate length scale for both simulation domains without compromising speed or accuracy. The flow leaving the outlets was used as the inlet flow condition for the room space simulations. Note that by doing so we essentially forced the duct simulation solution onto the room simulation. It was implicitly assumed that room air turbulence levels had no significant impact on the air/refrigerant mixture leaving the duct outlets.

For floor duct with standard 4-min leak and unit fan off (cases 1 and 5), the refrigerant dispersion through the duct network is slowed due to gravity. As such, essentially no refrigerant was shown to enter the rooms within the 10-min simulation time span. The refrigerant remained in the ducts resulting in a large flammable volume relative to the total duct volume. This combination of high flammable volume within the confines of the ductwork represents a significant fire risk if an ignition point is introduced (e.g., sparking when the system fan turns on). Note that this represents a worst case since no leakage from the ducts to surrounding ambient was assumed for these simulations. In a real case it can be expected that the refrigerant remaining in the duct will eventually escape to the crawlspace or attic and disperse to the outdoors. Still, for a fairly tight, low-leakage duct system, these results indicate a significant likelihood that a flammable volume could persist inside the ductwork for an extended time. The risk could be reduced by including a refrigerant sensor in the AC unit coupled with controls to start the unit blower in event refrigerant concentration above a set point (e.g., >25% LFL or other) is detected.

In the case of the ceiling duct, case 2, gravity enhanced the flow of the refrigerant. The maximum predicted concentration of the refrigerant inside the duct was ~14% in the vicinity of the leak release point, just below the R-32 LFL concentration.

For the room air flow simulations, underfloor ducts with fast leak and AC unit fan off using R-32 showed that the refrigerant volume fraction inside the room was extremely small; the maximum concentration was <0.01% in the space directly above the air grill. With the AC fan on and fast leak time, and AC indoor fan on, the maximum R-32 concentration within the space was ~5.3% (37% of LFL) at points just above the supply registers closest to the AC unit. After the leak end, the fan quickly dispersed the refrigerant throughout the room and refrigerant concentrations ranged from 0.5 to 1.0% at the monitored locations.

Results for Case 2, representing ceiling supply air ducts using R-32, showed that during the leak event (first 240 s), the refrigerant was entering the domain; while afterwards, the refrigerant mass flow rate through the diffusers decayed and eventually reversed directions within 1 and 2 s for outlets 1 and 2 respectively. Just before the leak ended, the R-32 concentration maximum is ~3.3% or about 23% of the LFL. At 241 s, room air began to flow into the supply registers while R-32/air mixture flowed into the hallway through the return grille. At 244s, the R-32 concentration near the return grille reached a maximum of ~2.9% (~20% of LFL concentration). At the 10-min point all the refrigerant was evenly dispersed throughout the space at ~0.4% concentration.

5.3.3 Single Room with Small RAC

This CFD simulation scenario focused on studying the leak from a small RAC with R-32 charge of 918 g (~3m^3 x R-32 LFL; LFL in kg/m^3) under four cases for different release heights and leak rates (Table 13, above). Simulations were performed to evaluate the volume fraction of R-32 inside a room (dimensions given in Figures 2 and 17). Six monitoring points (two each at 0.3m, 0.9m, and 1.5m elevations) were used for checking the refrigerant concentration. For case 1, the maximum volume fraction was around 4% (~28% of the R-32 LFL concentration of 14.4%) at the 0.3 m monitoring points at the end of the leak time. The volume fraction gradually increased during the leak event at all monitoring points due to the slow leak rate (550.8 seconds to leak the total charge). For cases 2 and 3, the maximum volume fraction was around 9% and 8% (about 63% and 56% of R-32 LFL) respectively at the 1.5 m elevation monitoring point closest to leak location. For both cases, it is observed that the volume fraction tends to gradually increase while the leak is occurring, then begins decreasing. Case 4 presents a leak from a 0.6 m height source. For this case, the maximum R-32 volume concentration was observed at the two 0.3 m monitoring points, reaching a value of ~7.3% (~51% of R-32 LFL) at the leak end point. This value is almost double the volume fraction seen for case 1 for the same leakage rate. The difference is attributed to the lower leakage location which affects the refrigerant dispersion inside the room. In none of the simulated cases did the refrigerant volume fraction at the monitoring points exceed the LFL value of R-32.

To further characterize the flammability risk for the simulated cases, the flammable volume (which is defined as the volume where R-32 volume fraction is between LFL and UFL) was integrated in space and presented in Figure 39, above. For a given release height (cases 1, 2, and 3, all at 1.8 m) the flammable volume size is proportional to the leak rate, while the residence time of the flammable volume is inversely proportional to the leak rate. The maximum flammable volume, ~3 liters, is seen for case 4 (slowest leak rate and low release height, 0.6m) while the minimum flammable volume, ~0.9 liters, is seen for case 1 (slowest leak rate and high release height, 1.8m). For case 4, the leaked refrigerant is released at a lower elevation which concentrates the refrigerant dispersion nearer the floor, which increases its volume concentration and accordingly the flammable volume. After the leak stops, the flammable volume dissipates as the refrigerant continues to mix with the room air. The flammable volume for all cases was observed close to the leak source at the wall.

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APPENDIX A.

PROJECT WORKSHOP ATTENDEES.

ORNL wishes to thank all of the workshop participants. The suggestions and feedback provided important insights about the research gaps and practical considerations of adoption of flammable refrigerants.

The workshop brought together 47 individuals from different entities across the industry. Table A 1 lists all the attendees and their affiliations.

Table A 1. Workshop attendees list

Attendee Name	Organization
Omar Abdelaziz	ORNL
Ahmad Abu-Heiba	ORNL
Masood Ali	Heatcraft Refrigeration Products
Tim Anderson	Hussmann
Pradeep Bansal	Satya International Ltd
Van Baxter	ORNL
Antonio Bouza	DOE
Brice Bowley	GE
Ahmed Elatar	ORNL
Thomas Frick	Manitowoc Foodservice
Brian Fricke	ORNL
Stephen Gatz	Whirlpool
Dave Godwin	EPA
Rakesh Goel	Lennox Industries
William Goetzler	Navigant
Siva Gopalnarayanan	Rheem
Clayton Grow	Convergent Science
Bill Hansen	Trane
Byron Horak	Intertek
Phillip Johnson	Daikin Applied
Steve Kujak	Trane
Richard Lord	Carrier
Beatriz Mibach	Coca Cola
Barbara Minor	Chemours
Ali Moghaddas	Heatcraft Refrigeration Products
Wayne Morris	AHAM
Nathan Mouw	Whirlpool
Jeff Newel	Hillphoenix
Paul Papas	UTRC
Viral Patel	ORNL
Vance Payne	NIST
Yi Qu	LBNL
Brian Rodgers	UL

Mike Saunders	Emerson
Marc Scancarello	Emerson
Michael Shows	Intertek
Chad Strickland	Electrolux
Dean Swofford	Hillphoenix
Rusty Tharp	Goodman Manufacturing
Jemsheer Thayyullathil	Viking Range
Dutch Uselton	Lennox International
Geethu Vasudevan	Friedrich
Mike Vaughn	ASHRAE, host
Xudong Wang	AHRI
Guolian Wu	Samsung Electronics America
Edward Wuesthoff	HTPG, Rheem Manufacturing
Jing Zheng	Consultant

APPENDIX B.

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