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Modeling Leaks of Flammable Refrigerants

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Hydrocarbons (HC) are being introduced as refrigerant in heat pumps and AC systems, as a part of the phase-down of synthetic refrigerants. As HC are highly flammable, standards are being refined for their safe use. To better understand the risks, computational fluid dynamics (CFD) can be used to determine the concentrations of flammable refrigerants during the release in case of a leak. In this article, we will give a brief overview of work done in the US, as well as provide examples of results which have been achieved using CFD in Europe. This work is part of the IEA HPT Annex 64 on Safety Measures for Flammable Refrigerants.

Introduction

Global warming requires phase-out of fossil fuels, and most countries are planning to be carbon-free by 2050. This requires decarbonization and electrification of the complete energy system. A large share of fossil fuels is used today for heating, in buildings, and industry. In the future, heating needs to be based on heat pumps instead, and the IEA has suggested that the installation of 600 million heat pumps is required by 2030 [1]. At the same time, synthetic refrigerants are being phased down, and in Europe, phased out completely for smaller systems, due to their high GWP and / or because they belong to the PFAS group of substances, of which many have been found to be harmful for the environment and for human health. For these reasons, there is broad interest in using natural refrigerants, and in particular, hydrocarbons are being introduced as environmentally safe alternatives. However, the flammability of these fluids needs to be taken seriously, and this is the topic of the IEA HPT Annex 64 on Safety Measures for Flammable Refrigerants. One of the activities within the Annex is investigating leakage scenarios, i.e., how flammable refrigerants (class A3) spread in a confined space in the event of a leak. In this article, we will present some findings, partly from our literature review and partly from the work within the Annex.

Findings from Investigations in The US

In the United States, A3 refrigerants, such as R290 (propane), have garnered significant attention as viable alternatives to high-GWP refrigerants due to their ultra-low global warming potential and excellent thermodynamic efficiency. These refrigerants offer a compelling pathway toward meeting climate goals by significantly reducing the carbon footprint of heating, ventilation, air conditioning, and refrigeration (HVAC&R) systems. However, the high flammability of A3 refrigerants, as designated under ISO 817 (also ASHRAE Standard 34), raises flammability concerns that necessitate rigorous and systematic risk assessment before widespread adoption. To this end, numerous U.S.-based studies and regulatory initiatives have focused on evaluating the associated flammability risks and developing protocols to ensure safe application.

In particular, the U.S. Department of Energy (DOE), in collaboration with national laboratories such as Oak Ridge National Laboratory (ORNL), has spearheaded experimental and modeling research to understand potential hazards and mitigation strategies. A comprehensive study by ORNL [1] examined refrigerant leak scenarios in both residential and commercial systems, demonstrating that the formation of flammable concentrations is typically localized and short-lived, especially when modern ventilation and leak containment strategies are employed. These findings underscore that the risk of ignition can be effectively managed through proper system design. The Air-Conditioning, Heating, and Refrigeration Technology Institute (AHRTI) further advanced this understanding through its Flammable Refrigerants Research Program. This initiative encompassed a wide range of real-world simulations involving leak ignition tests, charge size validation, and ignition source mapping in diverse room configurations. The resulting data confirmed that adherence to charge size limitations and the elimination of nearby ignition sources substantially mitigates flammability risk [2]. Similarly, Underwriters Laboratories (UL) responded to these findings by updating UL 60335-2-40, incorporating specific provisions for equipment using A3 refrigerants [4]. The revised standard mandates enhanced construction features and defines charge thresholds that help ensure safe deployment in residential and light commercial settings.

Complementing these empirical efforts, the National Institute of Standards and Technology (NIST) developed detailed computational models to quantify ignition probability and evaluate thermal consequences following a refrigerant release. Lemmon and McLinden [4] concluded that, under standard ventilation conditions and with proper leak detection technologies in place, the likelihood of ignition is minimal. These insights have been instrumental in shaping risk-informed design practices. ASHRAE's ongoing research projects, such as RP-1806 and RP-1839, have also provided critical data on ignition thresholds and flame propagation behaviors specific to A3 refrigerants [5]. The results reinforce that while flammable, these substances can be safely managed within confined environments, provided there is robust adherence to design codes and ventilation standards.

Finally, the U.S. Environmental Protection Agency (EPA), through its SNAP (Significant New Alternatives Policy) Program, has facilitated the conditional approval of A3 refrigerants like R290 in various end-use applications. Rule 23 [7] outlines specific use cases and safety conditions under which A3 refrigerants are deemed acceptable substitutes. Taken together, these research findings and policy developments reflect a growing consensus that A3 refrigerants, despite their flammability, can be integrated safely into RACHP (Refrigeration, Air Conditioning and Heat Pump) systems when supported by engineering best practices, updated safety standards, and continued innovation in leak detection and system architecture.

Examples of recent CFD studies

Two recent articles demonstrate clearly what results can be achieved by using CFD (Computational Fluid Dynamics) simulations to determine the hydrocarbon concentrations in a confined space after a leakage [8],[9]. Some of the results are presented here.

The simulations were conducted using ANSYS FLUENT 2023, employing the finite volume method with a second-order upwind difference scheme. The COUPLED algorithm resolved the pressure-velocity coupling, and turbulence modeling utilized both the standard k-epsilon (kε) and SST k-omega (kω) models. After validation against experimental data from Colbourne and Suen [10], the SST k-omega model was selected.

To examine refrigerant dispersion during unintentional leakage, simulations were performed in a small room with dimensions of X: 3 m, Y: 2.5 m, and Z: 3.5 m, with the AC unit mounted at y = 1.8 m on the middle of the wall (z = 0).

Refrigerant leakage was assumed from a hole on the right-hand side bend of the indoor unit (IDU) coil, occurring at a constant mass flow rate, as in the study by Colbourne and Suen [10]. The leaked refrigerant mixed with return air inside the IDU and was expelled with an average velocity of 1.3 m/s and a flow rate of 0.053 m^3/s.

According to IEC 60335-2-89, as can be seen in Figure 1, at a saturation temperature of 35°C, the leakage rate of R290 (propane) is 2.73 times that of R600a (isobutane). This results in R600a taking longer to fully discharge.

Across all pairs, R290 consistently shows higher concentrations than R600a, as can be seen in S1, S3, S5, and S7, with more intense and widespread gradients. When the fan is operational (S1, S2, S5, S6), refrigerant dispersion increases, reducing localized LFL percentages compared to scenarios without fan operation (S3, S4, S7, S8). The fan aids in mixing leaked refrigerant with room air, preventing high concentrations near the source. Conversely, when off, the refrigerant accumulates near the floor, increasing localized flammability risks.

Scenarios S7 and S8, where the IDU is at floor level and the fan is off, show the highest flammable volumes due to refrigerant settling. In contrast, when installed at a standard height (S5, S6), refrigerant disperses more before settling, reducing flammable volumes.

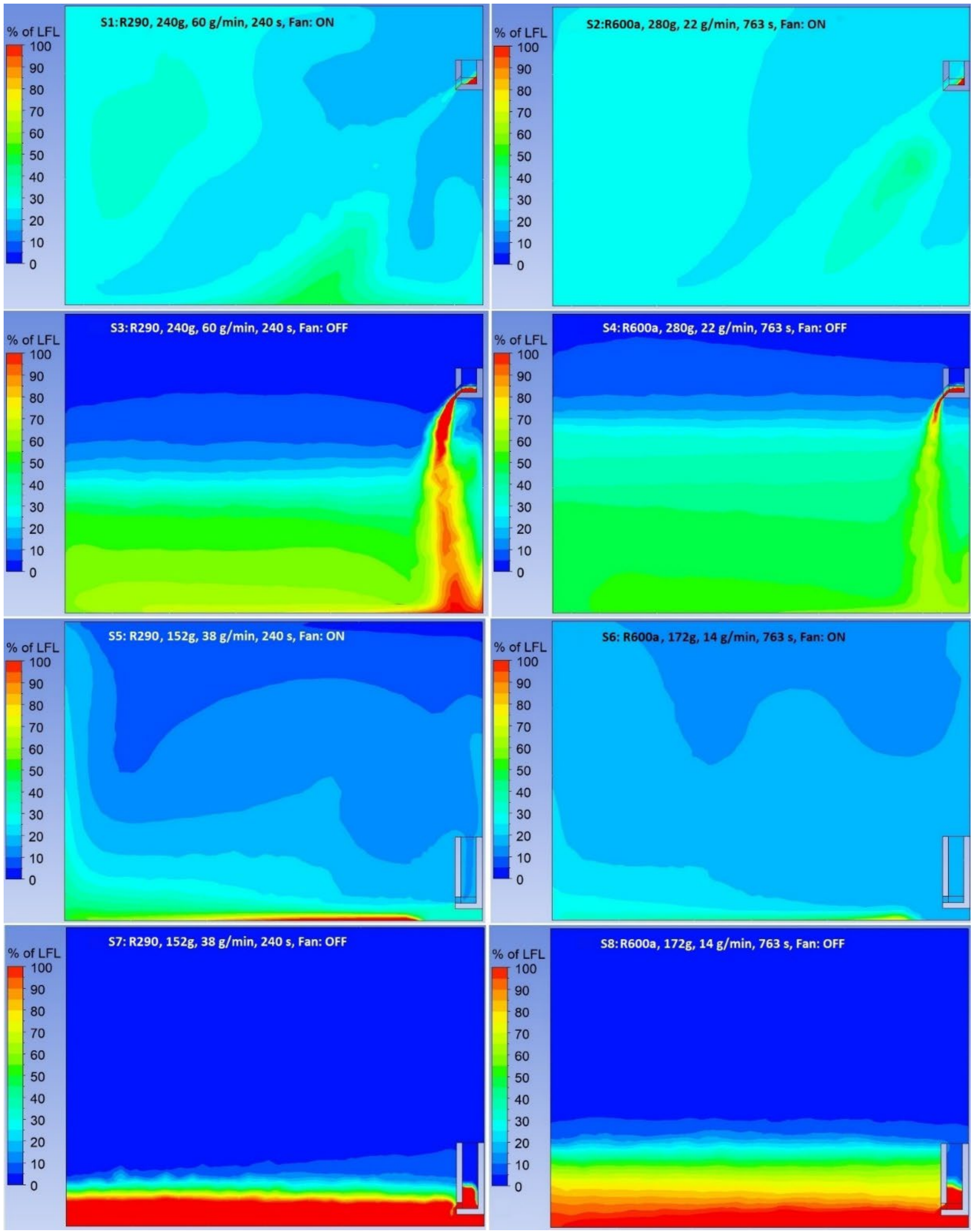

Figure 1: Refrigerant concentration contours after complete leakage. The middle plane was chosen for visualization to provide a comprehensive representation, though the highest concentration is in the leakage plane on the right side of the evaporator. Some regions exceed 100% of the lower flammability limit (LFL), but a 0-100% range was used to ensure comparability. The deepest red shade indicates concentrations surpassing 100% of the LFL.

Colbourne has published several papers on simulations of leakage scenarios. In an unpublished report, he shows that the maximum limit of 26xLFL, corresponding to 1 kg of propane, mentioned in IEC 60355-2-40 has no rational basis. A CFD model is used to demonstrate this. The model has been validated as reported in [10].

Here we will present the results only for an "unventilated" case, i.e., release under quiescent conditions. The indoor unit is installed at a height of 1.5 m, rooms are sealed except for an opening on the ceiling for relief of excess pressure due to introduction of refrigerant (although this is not included for consequence calculations).

Two leak rates were used, being instantaneous releases of 60 g/min and 180 g/min of propane. A series of CFD calculations were carried out to generate flammable volumes, flammable mass, and flammable times. For each set of conditions, several cases ranging up to about 4 kg were calculated and best fit curves plotted to enable a smooth estimation across the incremental increases in refrigerant quantities and room sizes.

Results for flammable volume vs time for the low and high mass flow cases are shown in Figure 2 and Figure 3, respectively. Generally, the flammable volumes for the high mass flow releases are about ten times those of the low mass flow. On the other hand, the time a flammable concentration persists is much shorter in the case of the large leak rate.

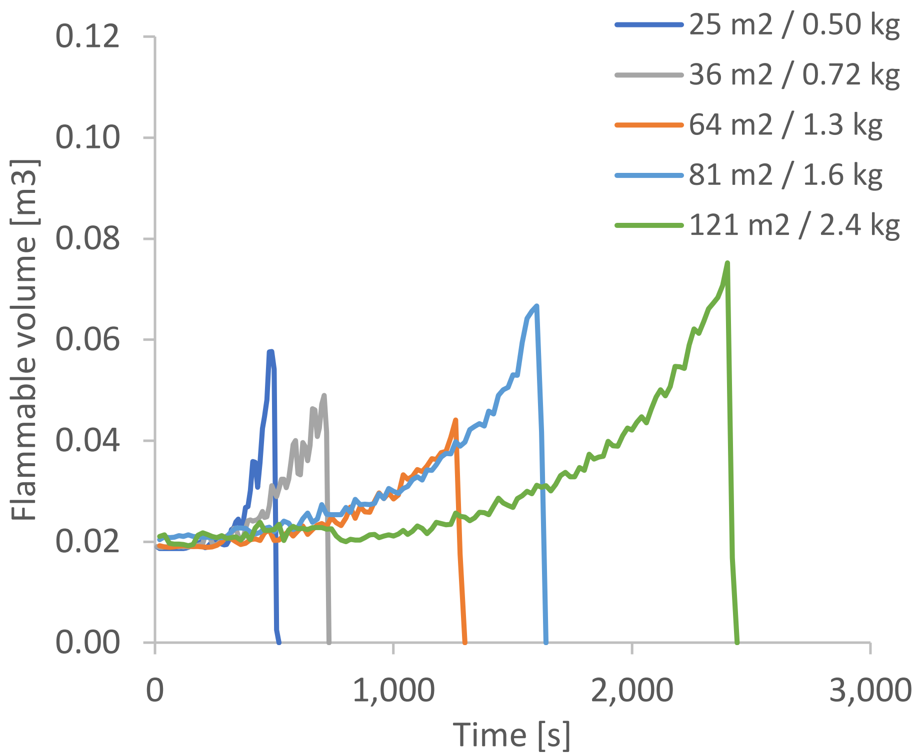

Figure 2: Flammable volume and time for low mass flow rate releases at 1.5 m unit height.

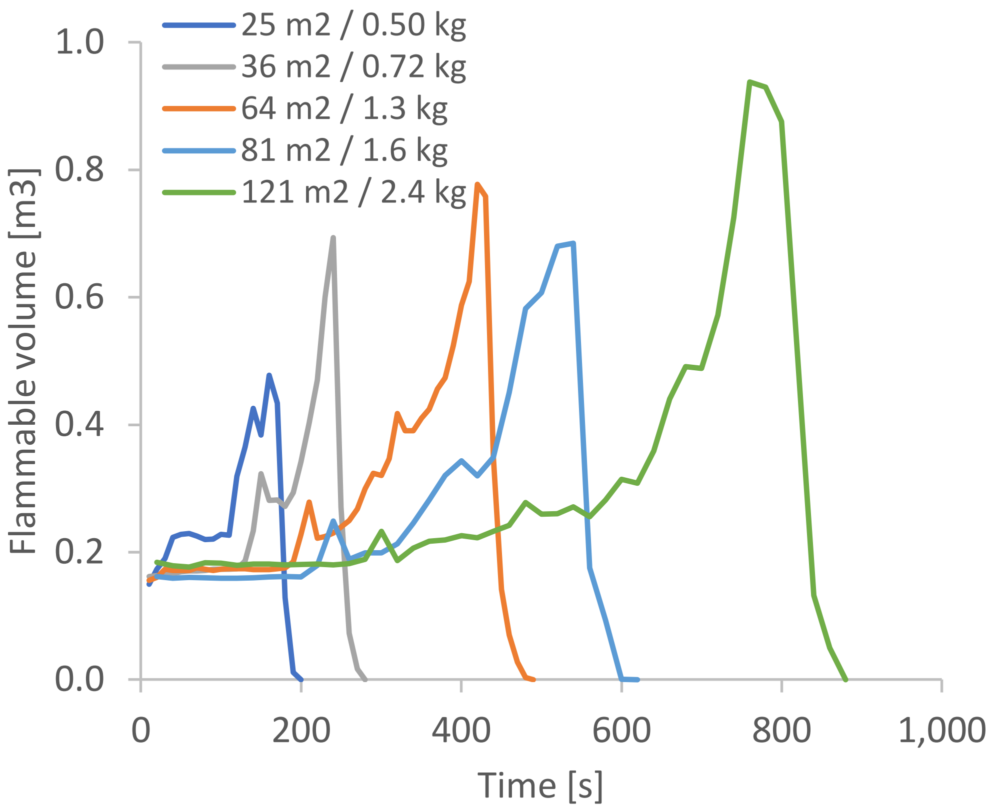

Figure 3: Flammable volume and time for high mass flow rate releases at 1.5 m unit height.

Conclusions

Determining refrigerant concentrations in a room after a leak of flammable refrigerant is important for understanding the risks. Numerical calculations, CFD, is an excellent tool for this purpose. Several reports and scientific papers have been published on this topic, publications which can be used as the basis when updating regulations and standards. In this article, we reported on some of the work done and gave a few examples of what type of results can be achieved. In particular, we showed that a leakage of isobutane (R600a) can be expected to give lower concentrations than propane (R290), leaking through a hole of the same size. We also showed the importance of having a fan in the room, and gave examples of how large the flammable volumes can be expected to be, and how long such volumes can be expected to exist, during leakages of different amounts of propane in rooms of different sizes.

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