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COMPLETION OF INITIAL REDUCED-ORDER MODEL FOR FLAMMABLE REFRIGERANT DISPERSAL IN RESIDENTIAL SPACES

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1. Introduction

Environmental regulations aimed at reducing global warming impacts of HVAC&R refrigerants have resulted in the phase-out of chlorofluorocarbons (CFCs) in 2010 and hydrochlorofluorocarbons (HCFCs) by 2030 in developed countries with additional restrictions on the use of hydrofluorocarbons (HFCs) set to take effect in 2036. Many of the remaining alternative refrigerants that have lower global warming potential (GWP) and that are suitable for use in HVAC&R systems (e.g., propane, difluoromethane) are flammable to some degree. Flammable refrigerants introduce new challenges and hazards to property and personal safety related to potential deflagration during system maintenance or due to leakage of the refrigerant accumulating in the conditioned space. Standards have been developed to set maximum charge limits for flammable refrigerants in HVAC&R systems; however, existing safety standards and codes still restrict their use. The bodies that maintain and update these codes need publicly available, science-based information to enable credible guidelines for setting safe charge limits for different flammable refrigerants in different HVAC&R applications. In 2016, 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 efforts to develop such information. As part of this effort, Oak Ridge National Laboratory (ORNL) began the current, ongoing project to examine imposed charge limits for flammable refrigerants and identify reasonable adjustments to these limits when found appropriate. Past tasks under this project have included development of experimentally vetted, computational fluid dynamics (CFD) simulation approaches to study the results of leakage of flammable refrigerants from various HVAC&R systems into different types of commercial and residential spaces.

In this report, we discuss recent efforts to develop a predictive model of the flammable volume fraction and accumulated refrigerant mass in a single-room residential space resulting from the leak of a flammable refrigerant from a small room air conditioning (RAC) unit. The eventual goal is development of a model suitable for public release which could simulate a range of scenarios. In discussions with the AHRTI Flammable Refrigerant Subcommittee (FRS) at the beginning of this effort, a total of 9 input parameters were chosen for consideration including room area, room/door opening area, ventilation fan flow rate, unit/leak height, leak area, leak rate, total refrigerant charge, refrigerant molecular weight, and state of the unit fan.

CFD simulations have proven to be capable of predicting the impacts of refrigerant releases into commercial and residential spaces with reasonable accuracy compared to experimental measurements. However, CFD approaches require expensive commercial software tools and considerable expertise to set up a model. Each CFD case then requires hours to days of computing time on high performance computing resources. As an alternative to delivering a CFD model, ORNL proposed an approach that uses results from CFD simulations to develop and train a reduced-order model (ROM) which contains the physics-based “knowledge” of the CFD model but is capable of simulating hundreds of scenarios in seconds. ORNL researchers have successfully used this approach for a variety of problems including simulation of cyclic variability in internal combustion engines.

This report details completion of the initial ROM development for a horizontal refrigerant release from the RAC unit into a single room with the unit fan off, on, or on after a delay (representing sensor detection of a leak and turning on of the fan to mitigate impact). Development of this initial ROM completes the FY2022 2nd quarter milestone for the project.

2. Approach

Our approach (shown schematically in Figure 1) begins with the development of a CFD model for detailed simulation of the refrigerant release from the RAC unit into the room. The CFD model is used to simulate several hundred to a few thousand individual cases with input conditions that span the multi-dimensional parameter space. Outputs from the CFD cases are processed to obtain the refrigerant concentration levels within the room as a function of time. This information can be used to reconstruct the flammable volume fraction and accumulated flammable mass of refrigerant within the room as a function of time for any combination of flammability limits. The inputs and outputs for the CFD training cases are then used to develop the ROM which consists of a set of continuous, differentiable mathematic relations for each output.

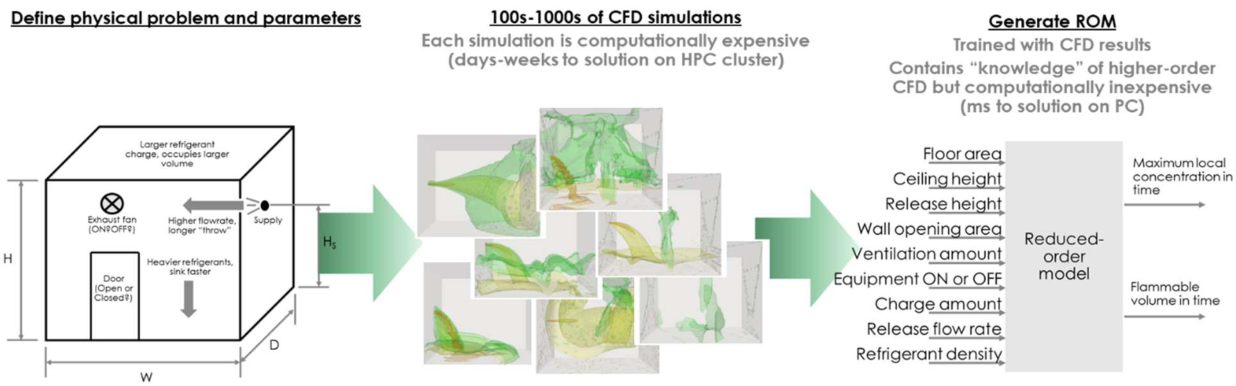

Figure 1: Schematic explaining our approach for development of the reduced-order model (ROM)

The CFD model was generated using the commercial code CONVERGE™ (v3.0). The model simulates release of refrigerant from a wall-mounted RAC unit into a single, symmetric room as shown in Figure 2. The geometry and input files were set up to enable bulk generation of the input file decks for each model case using bash scripts. The model uses a cubic base grid of 0.1 m (4 in) with adaptive meshing to reduce grid size automatically, down to a minimum of 12.5 mm (1/2 in) in regions of the domain where sub-grid differences in velocity or refrigerant concentration exceed 0.1 m/s or 0.01%, respectively. This embedding approach typical results in 0.5 to 1 million cells for the training cases. Turbulence is modeled using a Reynolds-Averaged Navier-Stokes (RANS) k-ε approach. Wall-time for the simulations varied depending on the input conditions but typically ranged from a few hours to several days (though a few cases required months to complete).

The RAC unit is modeled as being flush with the wall with the leak at the center of the unit air supply grill. The supply and return are modeled as inflow and outflow boundaries, respectively, with the same flow area (4 in x 20 in) and 1 m/s supply velocity. When the unit fan is on, the composition of gases leaving the room through the return is used set the composition entering the room through the supply to ensure conservation of species within the unit. The exhaust fan is modeled as an outflow boundary with a specified flow rate based on the value of the ventilation rate input parameter. Room doors are modeled as multiple flow boundaries with atmospheric back pressure which can be turned on or off to vary the open area from fully open to closed with only an air gap below the door. Any backflow into the room through the door opening is assumed to be fresh air. Each model run covers 15 min (900 s) of simulated time.

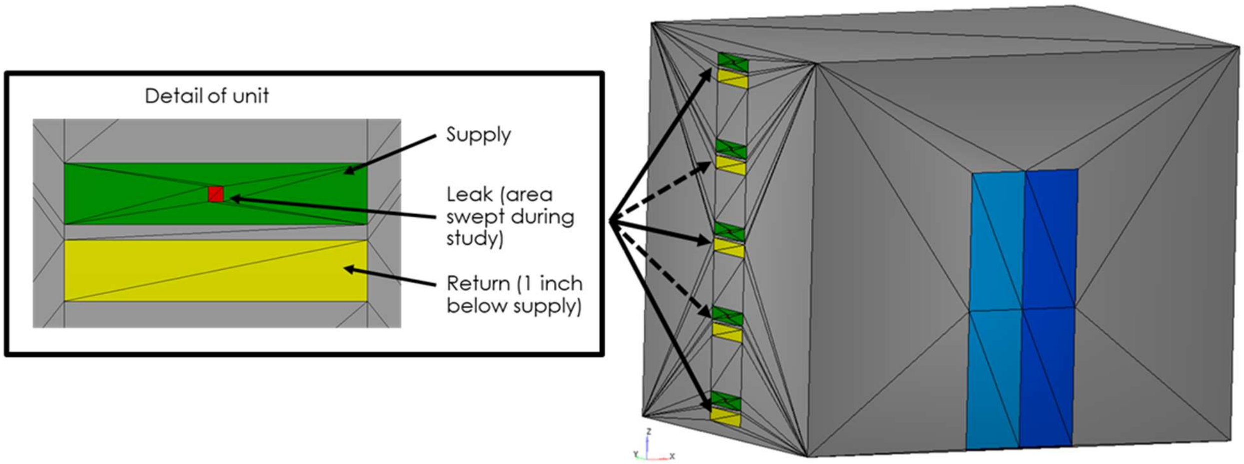

Figure 2: Example geometry model for the medium room size showing details of the flow boundaries used to model the RAC unit.

Table 1 provides the range and sampling points chosen for each of the nine input parameters considered in this study. An initial scoping study was performed to evaluate the sensitivity and functionality of the model response to each input parameter independently. Three sampling points were chosen for parameters with mostly linear responses including room area, door opening area, leak height, total charge, and leak rate. Molecular weight of the refrigerant and ventilation flow rate produced highly sensitive, nonlinear responses, thus more sampling points were used. Five sampling points were selected for the leak area parameter, but efforts focused on two values, 1 and 16 in^2. A full design-of-simulation approach for this parameter set would require 218,700 CFD simulations. Using a combination of sparse-grid sampling techniques and manual selection for additional focus in areas of high sensitivity or high flammable volume fraction, an initial set of 1816 input combinations were selected for training the ROM. Simulations were performed on the CADES high-performance computing (HPC) cluster at ORNL.

Results from the CFD simulations include refrigerant concentration in each cell of the domain at every second of simulated time. Post processing this data generates 482 output values selected to provide information on concentration levels and accumulated mass of refrigerant in the room as a function of time. Thirty-nine of those outputs form a matrix providing the minimum, mean, and maximum refrigerant concentration in the room as a function of time. Another matrix contains 221 output values describing the volume fraction of the room as a function of concentration level and time. This information can be used to determine the flammable volume fraction in the room as a function of time by interpolating within the matrix to obtain the volume of the room with refrigerant concentrations between the upper and lower flammability limits. A similar set of 221 output values form a matrix of refrigerant mass for determining accumulated flammable mass with the same approach.

The ROM is generated from the compiled inputs and outputs of the CFD simulations using the TASMANIAN (Toolkit for Adaptive Stochastic Modeling and Non-Intrusive ApproximatioN) toolkit developed by ORNL. TASMANIAN uses regression-based machine learning techniques to develop a continuous, differentiable mathematic function representing a multi-dimensional response map for each of the 482 model outputs over the 9 input parameters. Because the CFD model results are used to train the ROM, it inherently contains the physics-based knowledge of the CFD model without actually having to solve the physics. Instead, producing results from the ROM for a new set of input parameters only requires solving the 482 regression polynomials. This can be done almost instantaneously on a PC rather than taking days on an HPC cluster with the CFD model. The accuracy of the ROM can be assessed by comparing predictions to CFD results for input parameter sets not included in the training cases. TASMANIAN also provides guidance on areas of the parameter space where the regression methods incur higher error. ROM accuracy can then be improved by adding more training cases in these regions of the parameter space.

Table 1: Input parameter ranges and sampling points

Parameter	Values								
Fan state	ON 0-s delay	ON 30-s delay	ON 60-s delay	OFF 901-s delay					
Room area, m^2 (3:4 aspect ratio)	2.5	10	54.6						
Leak area, in^2	0.25	1	4	9	16				
Door opening, %open	0	50	100						
Exhaust ventilation, cfm	0	147	295	442	590	737	885	1032	1180
Leak height, % of ceiling	10	30	52						
Charge, lb	0.33	5.79	11.24						
Leak rate, lb/min	1.1	6	11						
Molecular weight, g/mol	44 propane	52 R-32	66 R-410, 452A, 454B	81 R-466A	120 R-1234s, R515s				

3. Milestone Progress and Results

In November 2021, with ~80% of the 1816 CFD cases complete, we performed an initial assessment of the ROM accuracy. The leak area parameter was found to be under-sampled in the initial set of cases with most of the simulations using a value of either 1 or 16 in^2 producing severe discontinuities in the ROM. To enable further analysis, the training cases were separated based on the value of the leak area parameter and then used to generate separate ROMs for small and large leak areas. The longer-term solution to this issue is to add additional training cases using intermediate values for the leak area input parameter.

Once separated into two ROMs, the overall accuracy of ROM predictions relative to CFD model predictions was found to be good, but with some areas of the parameter space identified as needing additional training samples. These comparisons were made using 14 cases with input parameter sets not used to train the ROMs. Six of the cases used the smaller leak area, and the other eight used the larger leak area.

Figure 3 compares CFD and ROM predictions for average refrigerant concentration in the room as a function of time for 3 of the 14 test cases (the data markers in the plots represent 13 of the 482 model outputs). For 8 of the 14 test cases (including case 10 shown in the figure), the ROM shows good to excellent agreement with the CFD model. The ROM overpredicts the average refrigerant concentration for five cases (including case 5 shown in the figure) while it underpredicts average refrigerant concentration for case 8. Despite these differences, the average error in concentration profile history is under 1% for all 14 test cases.

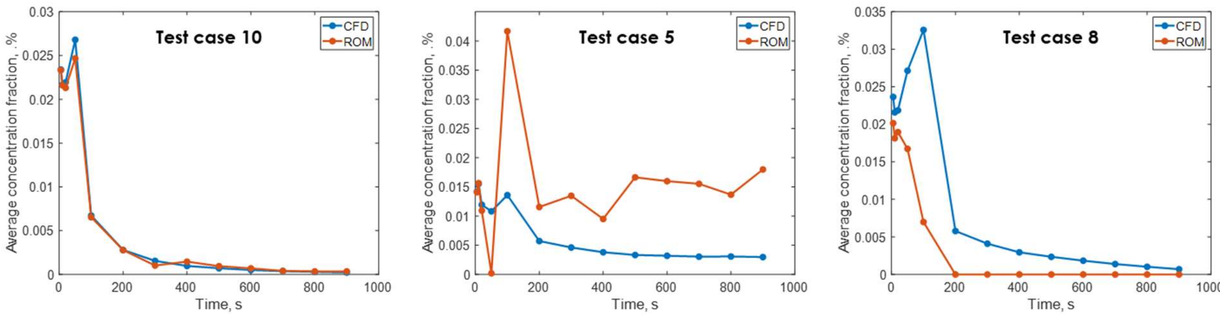

Figure 3: Comparison of average refrigerant concentration (i.e., molar fraction) predicted by the CFD model and ROM for three test cases.

Figure 4 shows similar comparisons for flammable volume fraction as computed using the flammability limits for propane (LFL = 2.1%, UFL = 10.1%) and R-32 (LFL = 13.9%, UFL 29.3%) and the matrix of 221 ROM outputs for volume fraction following the approach described earlier. When this matrix is generated using CFD outputs, each value in the matrix (and its error) has a physics-based connection to that of its neighbors. However, the values in a matrix generated with ROM outputs are discrete in nature with no physical or mathematical relation to its neighbor values. This allows introduction of discrete, compounding error into the flammable volume fraction profiles reconstructed using the ROM data.

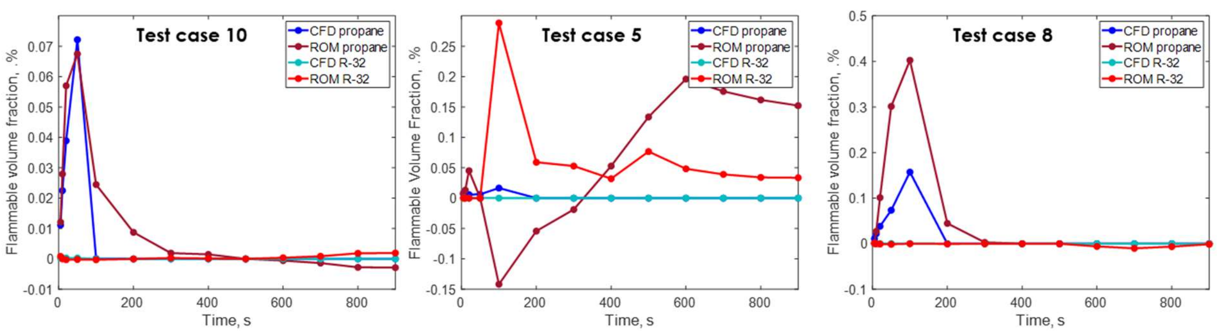

Figure 4: Comparison of flammable volume fraction (based on flammability limits for propane and R-32) predicted by the CFD model and ROM for three test cases.

As with the concentration profiles, the ROM predictions of flammable volume fraction agree well with the CFD results for a majority of the test cases (including case 10 shown in Figure 4). For some cases, however, the discrete errors introduced by the ROM lead to significant errors. For case 5, higher discrete errors near the upper flammability limit for propane result in negative flammable volume fraction predictions early in the simulation followed by over predictions of flammable volume fraction relative to the CFD results after 400s. Case 8 underpredicted the average concentration profile (Figure 3), but overpredicts the flammable volume fraction due to higher discrete errors near the lower flammability limits in the volume fraction matrix. Because the errors in the volume fraction matrix are discrete, increasing the number of ROM outputs to increase the resolution of the matrix is not expected to improve accuracy. Instead, additional training cases need to be added in these portions of the parameter space to improve the fit.

Based on this initial analysis, additional training cases were added to increase sampling in areas of the parameter space where the ROM accuracy was lower than desired. Several hundred cases were also added with leak areas between 1 and 16 in^2 to reduce the discontinuities in this parameter and alleviate the need to produce two ROMs.

The 1816 initial CFD simulation cases plus an additional 1111 cases to further refine sampling were completed in February 2022. The CFD results have been processed and used to generate a ROM meeting the intended goal of the FY2022 Q2 regular milestone: "Complete development of the first ROM". An analysis of the ROM accuracy (similar to that presented above) is in progress, and results will be presented to the AHRTI FRS in March 2022 and included in a future publication.

4. Next steps

Assessment of the current ROM's accuracy is ongoing. Based on the outcome of that assessment, completion of additional CFD training cases may be needed to further refine sampling in some portions of the parameter space. Once completed, results will be documented in a future publication (FY22 Q3 milestone for draft).

Based on discussions with the AHRTI FRS at the beginning of this project, the second priority for study is determining the impact of a vertical downward release of refrigerant from the RAC unit (compared to the horizontal release used in the current study). Remaining project resources will be used to assess this impact through completion of additional CFD simulations. The goal of this effort is to determine if the results are similar enough that a vertical release could be incorporated as an expansion of the current ROM or are too dissimilar necessitating the creation of a new ROM. There is a FY22 Q4 milestone for completion of this assessment.

5. Acknowledgements

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