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# APPLIED METHODS FOR ASSESSING FLAMMABILITY RISKS OF HFO REFRIGERANTS

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## ABSTRACT

Manufacturers worldwide are developing substitutes for refrigerants with high global warming potential (GWP) to address climate change concerns. Since 2007, we have used fault tree analysis (FTA) and Computational Fluid Dynamics (CFD) modeling to evaluate the safety of mildly flammable hydrofluoroolefin (HFO) refrigerants in the automotive and stationary sectors, an approach that has proven acceptable to several regulatory bodies. In this paper we will describe the overall approach we have used, illustrated by several case examples involving HFO refrigerants (*e.g.*, HFO-1234yf and HFO-1234ze(E)). This includes a description of open source CFD software to assess and visualize refrigerant dispersion. We also discuss the challenges of FTA parameterization when quantitative data are scarce, particularly as regards human factors. Finally, we share our experience using probabilistic tools for evaluating FTA uncertainty and comparative approaches for placing risks in context for the benefit of regulatory authorities.

Keywords: Computational Fluid Dynamics (CFD); Fault Tree Analysis (FTA); Flammability; Risk Assessment

## 1. INTRODUCTION

The Montreal Protocol (UNEP, 2017) mandated reductions in the use of ozone-depleting chlorofluorocarbons (CFCs) to mitigate damage to the Earth's ozone layer caused by chlorine in the stratosphere (World Meteorological Organization, 1998). Following ratification of the Protocol, hydrochlorofluorocarbons (HCFCs) were used as transitional replacements for CFCs owing to their lower ozone-depletion potential (ODP) and global warming potential (GWP; ASHRAE, 2017), with global production and consumption of HCFCs set to cap and then decline starting in 2004 (UNEP, 2017, Article 2F). Hydrofluorocarbons (HFCs) were used as replacements for HCFCs because they do not contain chlorine, and thus have an ODP of essentially zero (ASHRAE, 2017). HFCs can have higher GWPs than HCFCs, however. The recent passage of the Kigali Amendment to the Montreal Protocol (UNEP, 2016) requires that HFCs, too, be phased out of production and consumption.

Hydrofluoroolefins (HFOs) have been developed as substitutes for HFCs. HFOs have essentially zero ODP and significantly reduced GWP relative to HFCs. HFOs present a greater flammability concern than several traditional HFCs, however. While R-134a has an American Society of Heating, Refrigerating and Air conditioning Engineers, Inc. (ASHRAE) safety classification of A1, indicating no flame propagation, HFOs such as R-1234ze and R-1234yf have ASHRAE safety classifications of A2L, indicating that they are lower flammability refrigerants with a maximum burning velocity of less than or equal to 10 cm $s^{-1}$ (ASHRAE, 2010).

The potential for a transition from refrigerants with no flammability to refrigerants with mild flammability has prompted industry groups and regulatory agencies to seek assessments of the risk of refrigerant ignition. Quantitative evaluation methods are needed to calculate risks and support data-driven decision-making. This paper presents a risk assessment approach employing fault tree analysis and consisting of the following steps: qualitative fault tree construction (Section 2.1); fault tree parameterization (Section 2.2), including Computational Fluid Dynamics (CFD) modeling (Section 2.3); and quantitative fault tree comparative analyses (Section 2.4). The experience of the authors in applying this approach and placing the results in context for regulatory agencies is discussed in Section 2.5.

## 2. RISK ASSESSMENT APPROACH

Fault Tree Analysis (FTA) is a deductive system analysis method that combines the probabilities of undesirable events using Boolean logic to calculate the likelihood of a particular event, *e.g.*, the risk of refrigerant ignition (US NRC, 1981). The undesirable event of interest is placed at the top of a structure that organizes the contributing events to show the different pathways by which the undesirable event of interest could occur. An example fault tree visualization is given in Fig. 1.

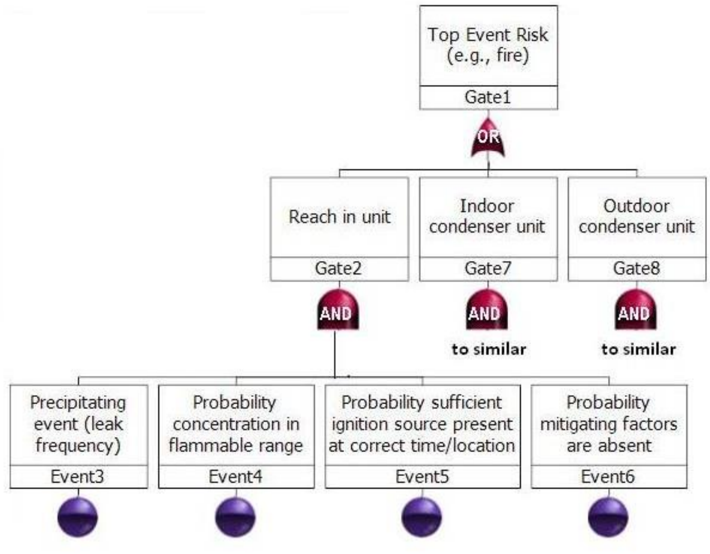

Figure 1. Example Fault Tree

The remaining sections of this paper describe the process by which FTA has been used to determine the risk of ignition of HFOs for industry groups and regulatory agencies. The overall assessment approach may be applicable to a broad range of refrigerant industry applications.

### 2.1 Qualitative Fault Tree Construction

A key first step in FTA requires envisioning all of the ways in which the undesirable event of interest might occur in order to create the fault tree structure. Visits to an example site and/or examinations of exemplary equipment that might be involved in an undesirable event are often helpful to contextualize potential risk and potential contributing events. Discussions with experienced professionals and reviews of the available literature can provide supplemental information. For example, a risk assessment for HFO in an end-use application could involve a visit to a facility currently employing the same end-use application, but involving a different refrigerant, and discussions with the current equipment operators to determine any prior events that may have indicated a risk, such as a repairman smoking indoors and setting off the building smoke alarms.

Examining all of the potential contributing events to an undesirable outcome is a qualitative process and prior assessments have required multiple iterations to develop a thorough characterization of the potential risk pathways. Typically, each iteration provokes new questions or uncovers additional factors that were not part of the original scenario concept. Given the "what if" nature of fault tree development, it is helpful to have professionals from a variety of backgrounds contribute to the development of the fault trees to gain as many unique insights as feasible.

Construction of the fault tree structure should incorporate all of the envisioned ways that the undesirable event of interest could occur, even if the probability of some contributing events is low or unknown. Careful consideration is also required to use appropriate logical structures to represent event occurrence. For example, HFO ignition is only possible if the HFO is present at flammable concentrations that spatially and temporally coincide with an ignition source, in the absence of mitigating factors that would prevent ignition; the mere presence of an ignition source and a flammable concentration does not alone guarantee HFO ignition if they do not occur at the same place and time.

### 2.2 Fault Tree Parameterization

FTA parameterization requires identifying or calculating numerical values for each contributing event developed as part of the qualitative fault tree development process. CFD modeling can be used to inform appropriate values to assign to key events that vary among use scenarios, namely the likelihood or probability that a flammable concentration is reached and coincides with a plausible ignition source in space and time. Parameters supported by CFD have typically been the most intensive to determine, but are also often of the most interest to regulatory authorities as they can be readily visualized and used as a communicative tool. An open source approach to CFD modeling that has been used in HFO risk assessments is described in Section 2.3.

Literature reviews and database queries are used to determine appropriate values for other parameters, such as equipment failure rates or leak frequencies. Original data collection in these areas has not typically been performed during the course of HFO risk assessments owing to the high cost of implementation. The Reliability Information Analysis Center publishes several databases, including the Electric Parts Reliability Database (EPRD) and Nonelectric Parts Reliability Database (NPRD) that represent compilations of failure rates for manufactured equipment and parts from the 1970s through 2013, with mathematical models provided to estimate reliability in areas where data are sparse (Quanterion Solutions Inc., 2014). In many cases, the databases helpfully provide information on the applications where part failures occurred, which allows researchers to assess whether the failure rates can be reasonably or conservatively applied to risk assessments of the equipment as used in other applications. Some manufacturers may have data on equipment failure rates, but such information is typically considered confidential and is difficult to obtain.

Inevitably, there will be inputs to the FTA where quantitative data are lacking. One approach to address such data gaps is by having guided discussions with subject matter experts to define the likely range of particular FTA input values. The set of experts should represent different perspectives on the scenario of interest, *i.e.*, different equipment manufacturers, component suppliers, and the experts should be encouraged to provide ranges of values that can be explored *via* sensitivity analyses. Human error rates, *e.g.*, failure to take a mitigation action or failure to perform a repair task correctly, are one particular factor that may be challenging to estimate. A number of references provide example error rates, which can be informative (*e.g.*, Blackman *et al*., 2008). Given the typically higher probability of human error relative to equipment or device failure rates, probabilities assigned to human factors should likely be examined *via* sensitivity analysis.

Iterative refinement of the FTA parameterization with experienced professionals is often necessary to ensure that the FTA is accurate for the application or applications of interest, erring on the side of conservative bounding values where refined information sources or data are unavailable.

### 2.3 Computational Fluid Dynamics Modeling

CFD uses numerical techniques to predict the solutions to the partial differential equations governing fluid dynamics, the Navier-Stokes equations (Munson *et al*., 2009, p. 318). CFD generally consists of designating a model domain, *i.e.*, a room or a finite outdoor area, and subdividing the domain into discrete control volumes in which conditions can be assumed to be uniform. The network of discrete control volumes is called the mesh, and a large number of mathematical techniques exist to divide a continuous geometry into a discrete mesh appropriate for use in CFD modeling (Owen, 1998). Common techniques used to discretize the model domain and mathematically represent the interactions between the cells comprising the mesh include finite volume, finite element, and finite difference methods. Resolving turbulent fluid flow phenomena in detail remains computationally expensive even using the aforementioned discretization techniques, and turbulence closure models are used to account for the terms of the Navier-Stokes equations that are not captured using averaging techniques. Common turbulence closure models include the Reynolds-averaged Navier-Stokes equations (RANS) and the large eddy simulation (LES) technique.

HFO risk assessments focus on the fluid effects of releasing an HFO refrigerant into a model domain otherwise occupied by air, such as might follow the occurrence of a leak in an otherwise hermetically sealed refrigeration or air conditioning device. The model domain is defined around the leak. For example, the domain for a leak in a walk-in cooler in a small commercial kitchen application could include the cooler, as well as the kitchen area outside the cooler and additional rooms further away from the leak. The definition of a domain larger than the immediate volume of interest may prevent unrealistic constraint of refrigerant dispersion. Where barriers to refrigerant transmission exist, *e.g.*, closed or sealed doors, representation of a larger domain area may not be necessary. The procedure to develop a model using the example of an HFO release from a walk-in cooler is described below, mimicking the walk-in cooler model from Air Conditioning, Heating and Refrigeration Institute (AHRI) Report 8009 (Gradient, 2015). The AHRI report included validation of the CFD results by experimental refrigerant release testing and monitoring.

A model domain and mesh was generated using the open source software Salome (Open Cascade, 2018). Salome provides a graphical user interface for construction of a model domain with a variety of options available to discretize the domain into a mesh that can be used for CFD modeling. The model domain is constructed by specifying the dimensions of volumes of varying permeability, *e.g.*, a box of impermeable walls inside which a refrigerant would be released. Fig. 2 shows a view of a model domain built using Salome. Complex geometries and interaction with other computer-aided design (CAD) software are supported. Once a continuous model geometry has been specified, the domain can be discretized into a mesh within the Salome program using several mesh generation options. Fig. 2 shows a tetrahedral mesh generated from the continuous geometric objects created in Salome with a maximum grid dimension size of 0.2 m and a minimum size of 0.01 m used to balance computational efficiency with results resolution. The geometric objects used to construct the domain can be grouped such that the control volumes associated with those objects in the mesh can be collectively referenced in the CFD model. For example, a geometric object associated with an air intake can be designated as a separate group, allowing the specification of an air inflow rate from the appropriate area in the CFD model. Exporting the mesh as a universal file format (UNV) file allows the mesh to be recreated and/or used by many other programs, including the open source CFD software OpenFOAM.

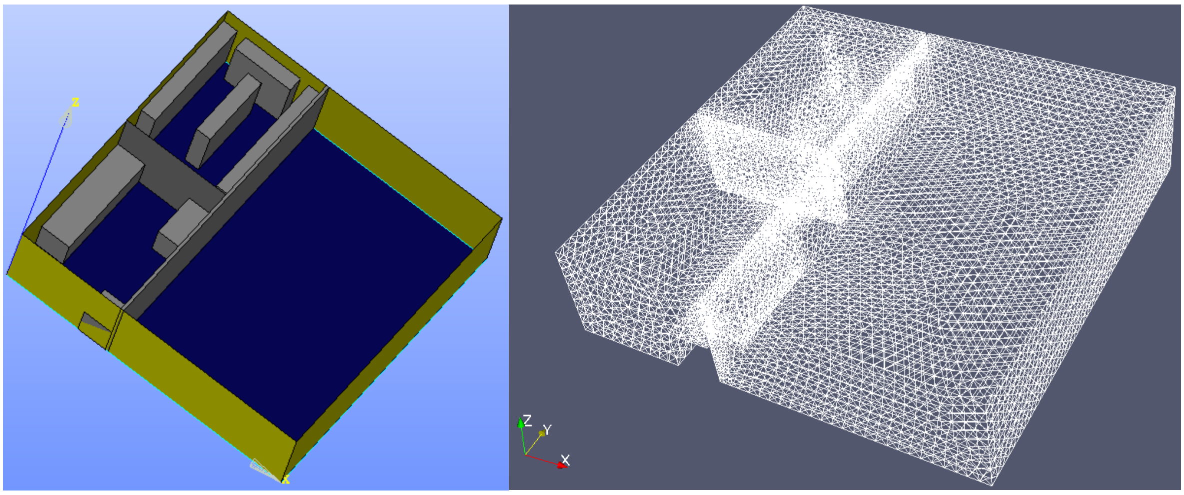

Figure 2. Model Domain for a Walk-in Cooler Constructed in Salome (left) and Salome-generated mesh (right).

OpenFOAM (Open source Field Operation and Manipulation) is a free, open source software for CFD designed as a programmable C++ toolbox (The OpenFOAM Foundation Ltd, 2018). Pre-programmed CFD solvers are capable of solving compressible and multiphase flow problems, and the open source development allows users to modify any aspect of the code if desired. Functionally, CFD simulations are simulated by specifying boundary conditions and material properties, and then using a CFD solver to numerically solve the system either in steady-state or as a function of time. Boundary conditions govern the mass and energy inputs and outputs to the system, as well as the initial conditions and spatial edge conditions. Boundary conditions specified for a CFD simulation would include a source of refrigerant mass and momentum at the location of a refrigerant leak, an initial state where the model domain is filled with air (as opposed to a refrigerant), and impermeable walls around the edge of the model domain. The properties of the refrigerant, including the density, viscosity, and other transport-related parameters must similarly be specified for a CFD simulation. The RefProp program (NIST, 2018) provides robust estimation methods for determining the properties of refrigerants and refrigerant blends from a database of known data. Leak rates can be calculated using analytical formulations for releases of gases from pressurized systems, including under choked flow conditions (Munson *et al*., 2009, p. 597-601). The parameters for a CFD simulation are specified in a series of text files read by OpenFOAM, and a simulation is executed by referring a CFD solver to the files specifying the boundary and property conditions. OpenFOAM supports parallel processing, leading to efficient simulation computational times; in the authors' experience, simulations have lasted on the order of hours to days on a 4-processor laptop. Outputs can be saved at user-specified time intervals and locations, including saving the entire domain status (*i.e*., the concentrations of the released refrigerant at every point in the domain) at a regular time interval from which the release distribution can be reconstructed. Pressure, temperature, air velocity, and other parameters can similarly be saved.

The results of the CFD simulations can be processed using a variety of data analysis techniques, since the results written to file are specified by the user and are written in standard formats. ParaView (Ahrens, *et al*., 2005) is an open source graphical user interface that can be readily used to visualize the results. OpenFOAM results can be converted to a Visualization Toolkit (VTK) format, which is the data processing and rendering engine relied upon by ParaView for visualizations. Practically, the CFD results can be converted to a VTK format using a single command that combines the refrigerant distributions for all simulation times. The VTK file can be read by ParaView and the results visualized with minimal processing time. ParaView offers the ability to customize the output by specifying color intervals for particular concentrations of interest or showing air pressure alongside the refrigerant distribution. Fig 3. shows an example of OpenFOAM CFD results visualized in ParaView.

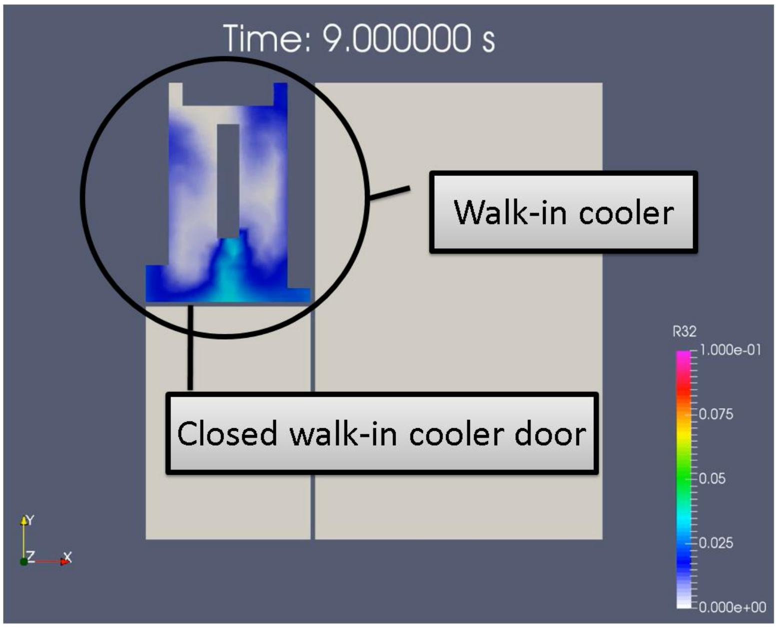

Figure 3. Visualization of OpenFOAM results using ParaView for a refrigerant released into a walk-in cooler with the door closed.

ParaView facilitates interpretation of the CFD results for the FTA by allowing the user to view only the portions of the dispersed refrigerant that are above the Lower Flammability Limit (LFL) and below the Upper Flammability Limit (UFL) in a 3-dimensional environment. The program can be used to estimate or calculate the amount of time that a refrigerant concentration is between the LFL and the UFL within a given area, which can be used to parameterize the fault trees.

The results of the CFD process outlined in Section 2.3 were compared to the experimental measurements presented in AHRI Report 8009 (Gradient, 2015) for multiple geometries and release scenarios. Concentrations at discrete monitoring points within the CFD domain showed good agreement with the experimental values (Fig. 4), and the overall patterns of refrigerant distribution were very similar to those presented in the modeling shown in the published report.

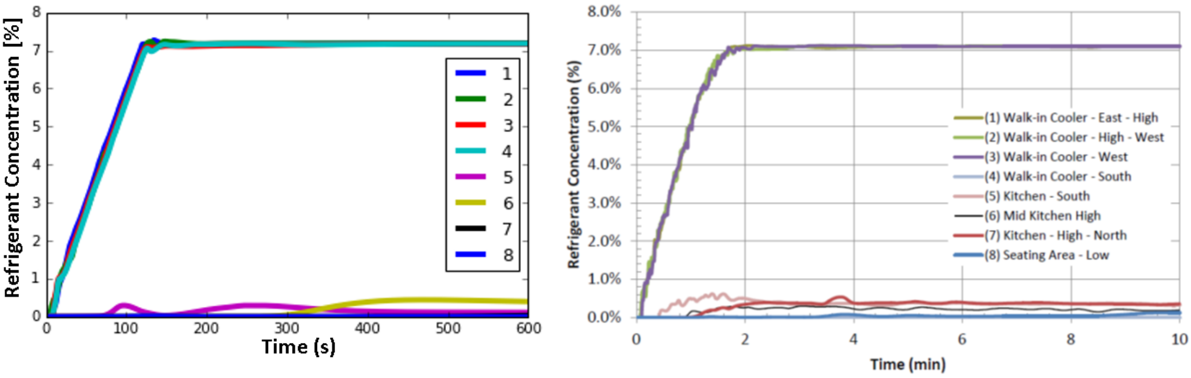

Figure 4. Comparison of R-32 concentrations at discrete monitoring points from CFD conducted with OpenFOAM (left) and results presented in AHRI Report 8009 (Gradient, 2015; right).

### 2.4 Quantitative Fault Tree Comparative Analyses

Calculating risks using FTA without values for comparison deprives the calculated risks of context. Risks are commonly accepted by the public as a natural part of society, including risks from hazards in the work place and commuting. Parameterizing fault trees and performing the calculations for an FTA can determine a numerical value for risk. Comparing the FTA-calculated value to the risk posed by existing refrigerants, or to common values of risk accepted by the public, is important to determine the relative incremental risk. For example, the FTA process performed for an HFO in a new application can be repeated for several alternative proposed refrigerants to determine which poses the least risk, and then evaluated in concert with other variables of interest, *e.g.*, GWP. Further, the risk of refrigerant ignition may be found to be substantially less than risks commonly accepted by the public, which may be of help to manufacturers and regulators seeking to determine what an acceptable level of incremental risk may be. Table 1 lists multiple risks commonly accepted by the public.

Table 1. Risks from Common Hazards or Hazards Related to Ignition

| Hazard | Risk (per year) | Source |
|---|---|---|
| Commercial building fire significant enough to warrant fire department response | $2 \times 10^{-2}$ | NFDC (2013) |
| Commercial building fire resulting from cooking activity | $3 \times 10^{-3}$ | NFDC (2013) |
| Injury at work due to fires or explosions | $2 \times 10^{-5}$ | US BLS (2016) |

### 2.5 Use Examples

The risk assessment approach described in the preceding sections has been used successfully for applications to the US Environmental Protection Agency's (US EPA's) Significant New Alternatives

Policy (SNAP) program and in other risk assessments for refrigerant manufacturers and users. HFO-1234yf and an HFO-containing refrigerant blend were evaluated for use in automotive air conditioning systems, both including a comparative evaluation of carbon dioxide (R-744) (Gradient, 2009; 2012). HFO-1234yf and HFO-1234ze(E) were also evaluated using a similar approach for stationary applications as part of AHRI Report 8009 (Gradient, 2015). In each case, some uncertainty has been present in the parameters used for the FTA. Probabilistic evaluations, such as Monte Carlo analyses, are adaptable to use with FTA and can be used to understand the range in possible risk values. The process of parameterizing the fault trees can, in fact, proceed by starting with the known or easily obtainable parameters, and then refining the estimates for the areas of highest uncertainty. This may eliminate the need for detailed analysis along branches of the fault trees that are not risk-driving, and may also provide upper bound risk values for the undesirable event of interest, if conservative values are used as placeholders until the input refinement is complete.

## 3. CONCLUSIONS

FTA provides a formal, quantitative framework for assessing the risk of an undesirable event of interest. The methods outlined in this paper provide risk assessors and engineers with a systematic way to use FTA for refrigerant risk assessments, incorporating CFD modeling and best practice methods for determining appropriate input probabilities under sparse data conditions. Open source and free or relatively inexpensive datasets and modeling tools have been recommended, where available, to facilitate broad method adoption.

## NOMENCLATURE

| | |
|---|---|
| AHRI | Air Conditioning, Heating, and Refrigeration Institute |
| ASHRAE | American Society of Heating, Refrigeration and Air Conditioning Engineers |
| CAD | Computer-aided Design |
| CFC | Chlorofluorocarbon |
| CFD | Computational Fluid Dynamics |
| FTA | Fault Tree Analysis |
| GWP | Global Warming Potential |
| HCFC | Hydrochlorofluorocarbon |
| HFO | Hydrofluoroolefin |
| LES | Large Eddy Simulation |
| LFL | Lower Flammability Limit |
| ODP | Ozone-depletion Potential |
| OpenFOAM | Open source Field Operation and Manipulation |
| RANS | Reynolds-averaged Navier-Stokes |
| SNAP | Significant New Alternatives Program |
| UFL | Upper Flammability Limit |
| UNV | Universal File Format |
| US EPA | US Environmental Protection Agency |
| VTK | Visualization Toolkit |

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