

# A MODERN TOOL FOR THE INVESTIGATION OF INDOOR FLAMMABLE GAS MIGRATION

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## ABSTRACT

When an accident, such as a fire or an explosion, occurs, the scientific method requires the investigator to evaluate all possible scenarios and determine which one (or more than one) is consistent with the available information – be it forensic evidence, witness testimony, and so on. One step in the investigation is the evaluation of potential leaks of flammable materials and of the dispersion of the resulting gas clouds within the region of interest. While simplified tools, such as mathematical correlations or zone models, are often used to test origin and cause hypotheses, a three-dimensional CFD simulation can provide additional details on the dynamics of the flammable gas cloud that cannot be captured by a simplified model.

This paper demonstrates the application of FLACS, a CFD model developed specifically for the simulation of gas dispersion and vapor cloud explosions, to indoor releases of flammable gases. The case studies presented in this paper demonstrated how relatively minor differences in the characteristics of the releases (e.g., the direction of the jet, or the momentum of the release) can have a significant impact on the growth of the cloud and, consequently, on the location of viable ignition sources as well as on the intensity of the resulting overpressures.

## BACKGROUND

Fires or explosions due to the ignition of a flammable gas leak within a structure are unfortunately common occurrences. In most of these cases, a critical part of the investigation consists of examining the gas supply system and identifying potential sources of gas leak. Oftentimes, due to the damage from the fire or explosion, several leaks are identified, in different locations and of different sizes. The scientific method requires the investigator to evaluate all available fuel sources for their possible contribution to the incident. This process involves estimating, for each possible source, the size, time development and spatial distribution of the resulting flammable cloud within the structure and reconciling the extent of this cloud with the location of potential ignition sources and fire damage.

There are several simplified investigative tools, such as mathematical correlations or zone models, which may provide useful information for this purpose and allow the investigator to eliminate some of the scenarios from consideration. However, these tools generally lack the sensitivity necessary to discriminate between similar – but not identical – scenarios and thus often result in an undetermined cause of the accident. For example, it is generally assumed that a natural gas leak will rise due to its buoyancy, so, if a natural gas leak is suspected to have occurred, investigators will typically look for potential ignition sources near the ceiling. However, the expected behavior of the gas cloud can be affected by several factors, such as: the characteristics of the leak itself (e.g., a high-momentum leak tends to mix with air more than a low-momentum leak), the presence of obstacles (e.g., furniture), air flow through doors and windows, temperature difference to outside or mechanical ventilation (e.g., HVAC vents and returns). The effect of these parameters on the gas cloud distribution is difficult to quantify accurately. As a result, investigators using simple tools may be unable to determine conclusively

which, among two or more potential scenarios, was responsible for the accident under investigation.

A more refined approach could be, for example, performing experiments that attempt to reproduce the postulated sequence of events. However, such experiments tend to be time-consuming and expensive and, in the case of indoor releases of flammable gases, may pose significant risks. A simpler but still accurate method to evaluate different gas leak scenarios is to use Computational Fluid Dynamics (CFD) models. These tools can provide spatially- and temporally-resolved quantitative information on the size, concentration and location of the flammable gas cloud from the occurrence of the leak to the ignition event. The investigator can then use this information to determine, for each potential scenario, whether the cloud may have reached viable ignition sources. Some CFD models, such as FLACS [1], can also provide quantitative information on the propagation of the flame front and on the overpressure distribution after the ignition of the cloud. The vapor cloud explosion dynamics predicted by FLACS can then be compared with forensic evidence, such as broken windows or other explosion-related damage, to further evaluate whether the postulated sequence of events is consistent with the available information. Several “what-if” scenarios can be run and compared against the evidence and against each other, with fine spatial and temporal resolution and in a fraction of the time and cost associated with experimental testing.

This paper will briefly describe the CFD model FLACS and then provide examples of its application to indoor leaks of propane and natural gas, to demonstrate the effect of leak location and momentum on the behavior of the flammable cloud.

## **THE FLACS CFD MODEL**

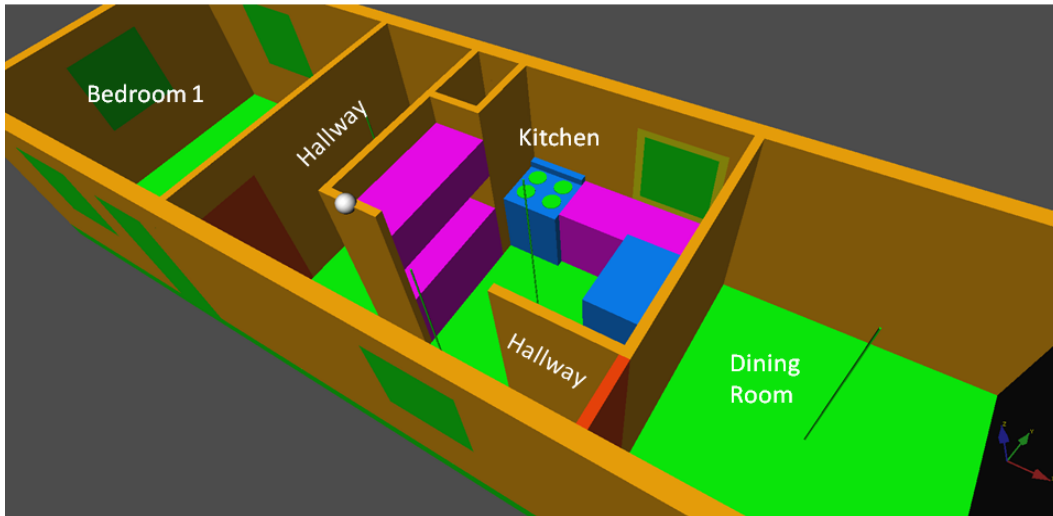
FLACS is a CFD tool developed since 1980 by GexCon for the simulation of gas dispersion and vapor cloud explosion scenarios. FLACS is capable of modeling gas and aerosol releases, dispersion of vapors, ventilation in structures, and ignition of flammable fuel-air mixtures to evaluate the flame front progression and the overpressures due to explosions. FLACS solves the compressible Reynolds-Averaged Navier–Stokes equations on a 3D Cartesian grid using a finite volume method and the  $k$ - $\epsilon$  turbulence model. The conservation equations for mass, impulse, enthalpy, turbulence and species, closed by the ideal gas law are included.<sup>1,2</sup> The FLACS code implements a “distributed porosity concept” which allows the detailed representation of complex geometries using a Cartesian grid: large objects and walls are represented on-grid, and smaller objects are represented sub-grid. This allows the effect of small obstacles to be accounted for, while maintaining reasonable simulation times:<sup>3</sup> sub-grid objects contribute to flow resistance, turbulence generation and flame folding in the simulation. FLACS contains a flamelet-based combustion model with one-step reaction kinetics, where the laminar burning velocity is one important measure of the reactivity of a given mixture. Flame acceleration is included, due to flame instability, flame-folding by obstacles and turbulent mixing.<sup>4,5</sup>

FLACS has been extensively validated against numerous gas dispersion<sup>6,7</sup> and vapor cloud explosion experiments,<sup>8</sup> including large-scale realistic release and explosion tests performed at GexCon as well as full-scale experiments performed in a semi-confined model of an offshore module.

## **CASE STUDY: PROPANE LEAK IN MANUFACTURED HOME**

The effect of leak momentum, direction and elevation for a negatively-buoyant release (propane, with specific gravity of approximately 1.5) were evaluated for a small manufactured home, as shown in Figure 1 using the FLACS geometry pre-processor CASD. The layout of the home was similar to the setup used by Schumacher et al.<sup>9</sup> for their indoor gas dispersion experiments. The

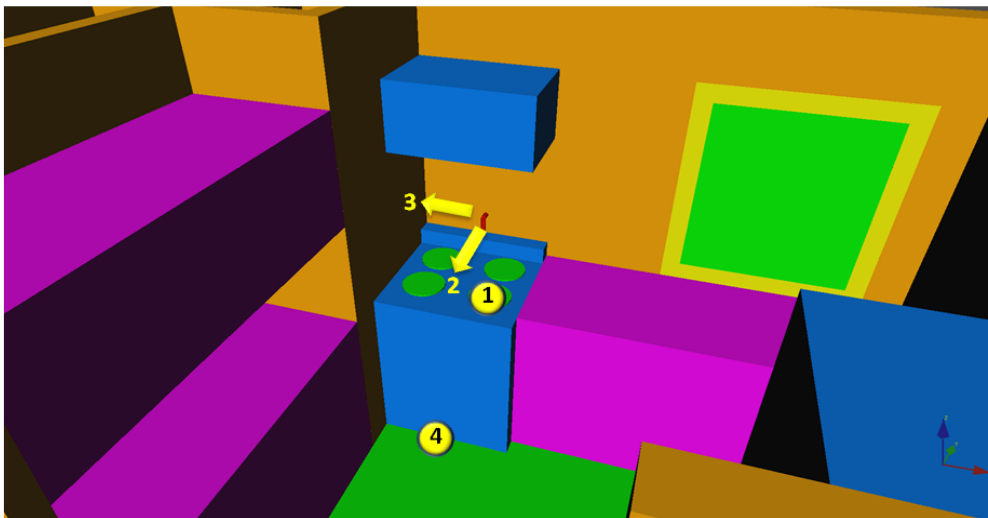
computational domain for the propane release simulations was limited to the kitchen, hallway and dining room; the doors to the two bedrooms (at both ends of the home) were assumed closed. Gaps for air and gas flow were assumed at the bottom of the two bedroom doors and around the perimeter of the kitchen window. Air flow into the home, due to external wind pressure, was imposed along the perimeter of the hallway window. The leak flow rate was approximately 1.3 g/s (2.57 m<sup>3</sup>/h) at ambient temperature (20°C) and pressure, and remained constant for one hour.



**Figure 1. Layout of the manufactured home, shown using CAD (ceiling removed for clarity).**

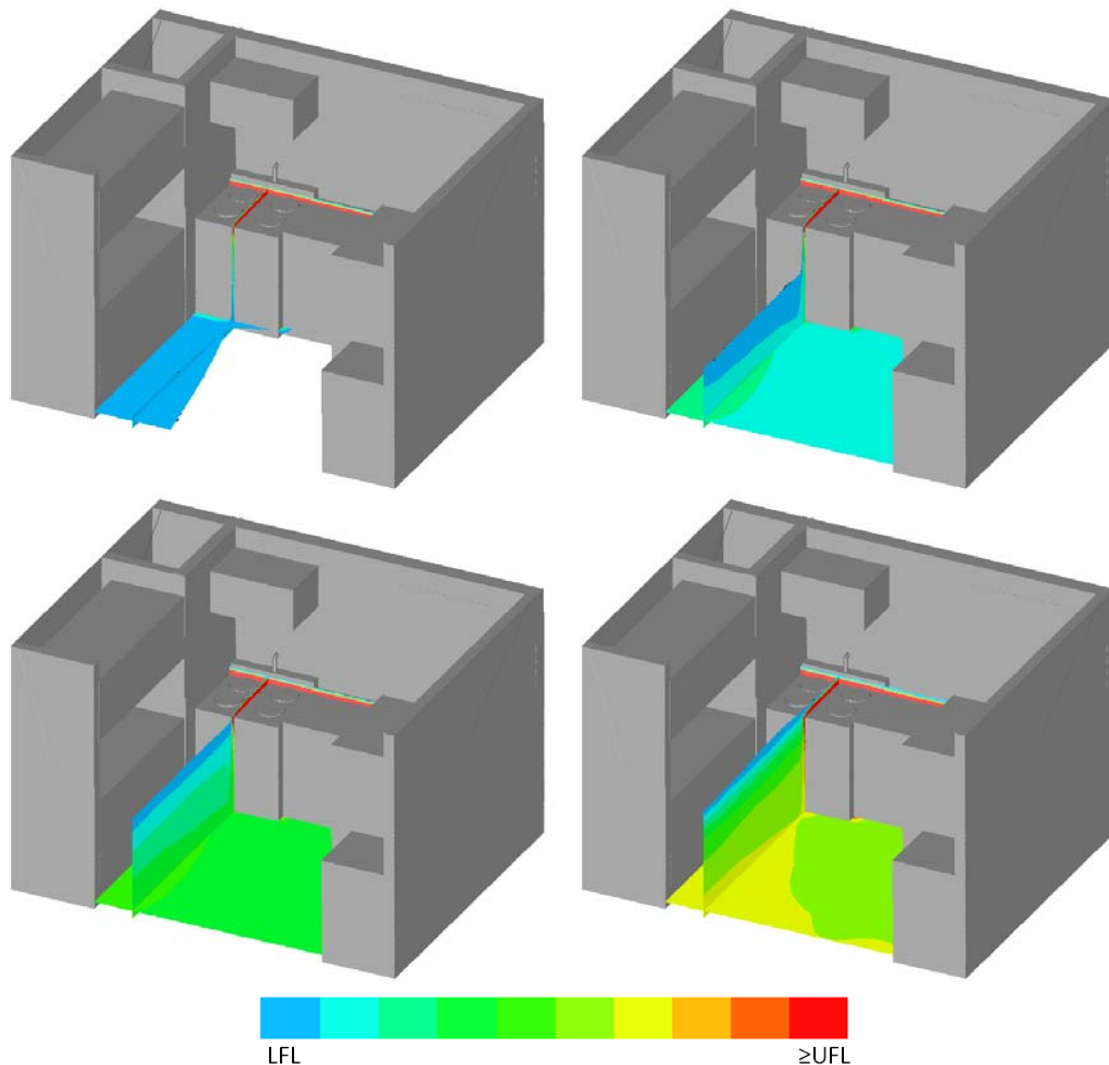
The following four propane release scenarios were compared, as shown in Figure 2:

1. Elevated diffuse release: a low-momentum leak from the front-right range burner;
2. Free jet: a high-momentum leak from a 3/8-inch diameter hole in the gas supply piping, originating approximately 23 cm above the range and directed away from the wall;
3. Impinging jet: a high-momentum leak from a 3/8-inch diameter hole in the gas supply piping, originating approximately 23 cm above the range top and directed parallel to the far wall, towards the wall to the left of the range;
4. Ground-level diffuse release: a low-momentum leak from the front of the range, originating near ground level (1 cm elevation).



**Figure 2. Release scenarios for the propane leak case study.**

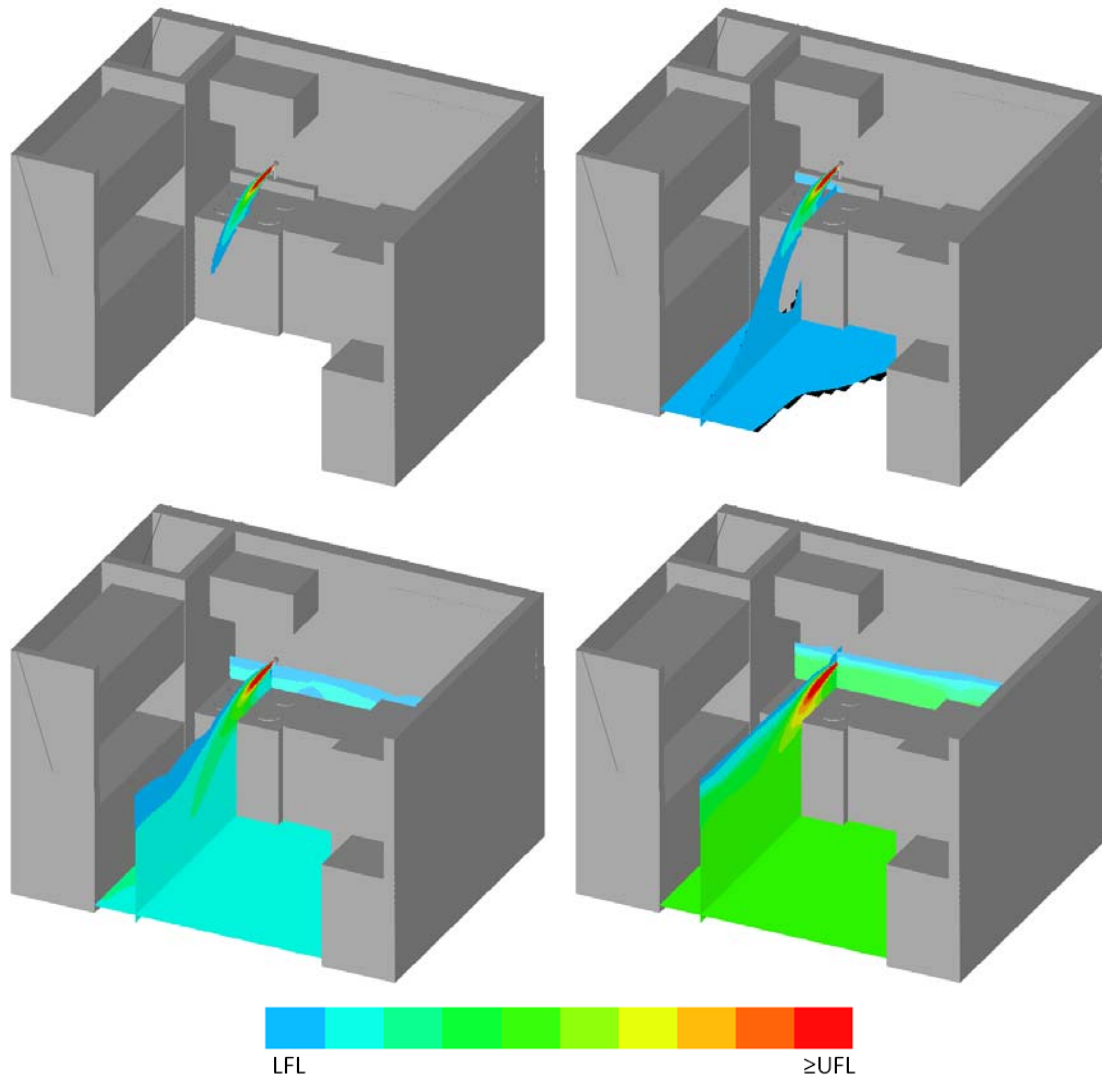
Figure 3 shows snapshots of the propane gas cloud formed by the release and dispersion of an elevated diffuse leak: the front-right burner on the kitchen range was assumed to be open and unignited. The time sequence shows the initial formation of a layer of gas (mostly at or above the upper flammable limit – UFL – which is approximately 9.1 mol% for propane) on the range and adjacent countertop surfaces. As the gas layer spills over the edge of the range, its weight causes it to drop to the ground; however, air entrainment during the fall significantly reduces the gas concentration in the ground-level layer, to the point where initially it is at or below the lower flammable limit (LFL, approximately 2.1 mol% for propane). As the leak continues, the countertop-level layer remains thin and rich, while the ground-level layer grows in thickness as well as gas concentration. The stratification within the ground-level layer is noticeable and indicative of poor mixing between the dense gas and the air.



**Figure 3. Propane cloud concentration from elevated diffuse leak, after: 5 minutes (top-left); 15 minutes (top-right); 30 minutes (bottom-left); and 60 minutes (bottom-right).**

The free jet release scenario (propane leak from a 3/8-inch diameter hole perpendicular to the wall) is shown in Figure 4. The propane jet exits the hole horizontally with a velocity of approximately 9.6 m/s. As shown in the top-left figure (5 minutes into the leak), the density of the jet rapidly turns it downward, however, the jet centerline overshoots the edge of the range.

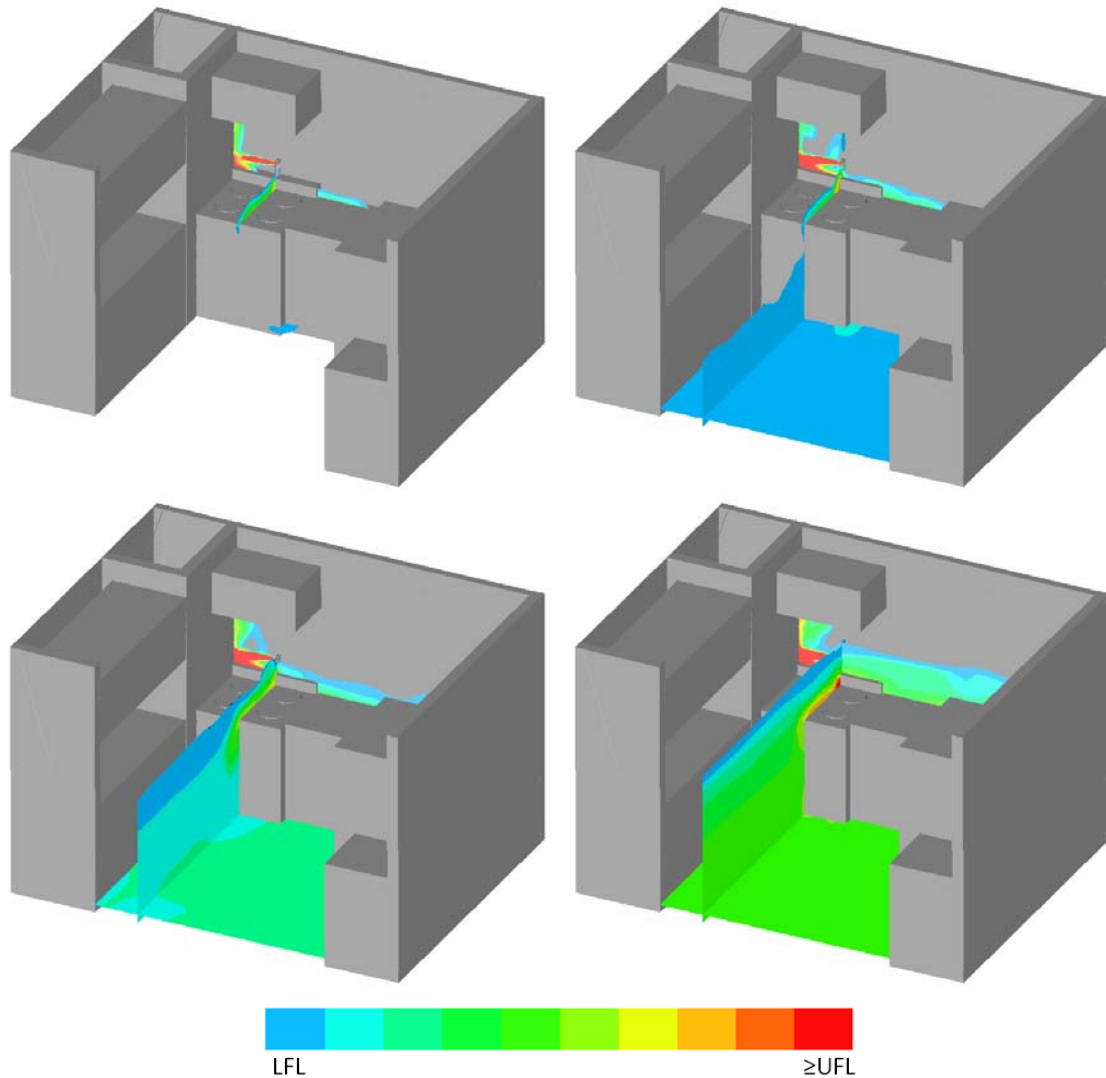
Therefore, only a fraction of the released propane accumulates on the range and countertop surfaces, resulting in a relatively thin layer but entirely within the flammable range. The air entrainment into the bulk of the jet results in a well-mixed cloud near ground level. As the leak continues, the gas concentration within the cloud increases while remaining relatively uniform due to the jet-induced mixing. After one hour, the kitchen volume from the ground to slightly above the countertops is filled with a well-mixed propane cloud at approximately stoichiometric concentration (4.3 mol% for propane).



**Figure 4. Propane cloud concentration from free jet leak, after: 5 minutes (top-left); 15 minutes (top-right); 30 minutes (bottom-left); and 60 minutes (bottom-right).**

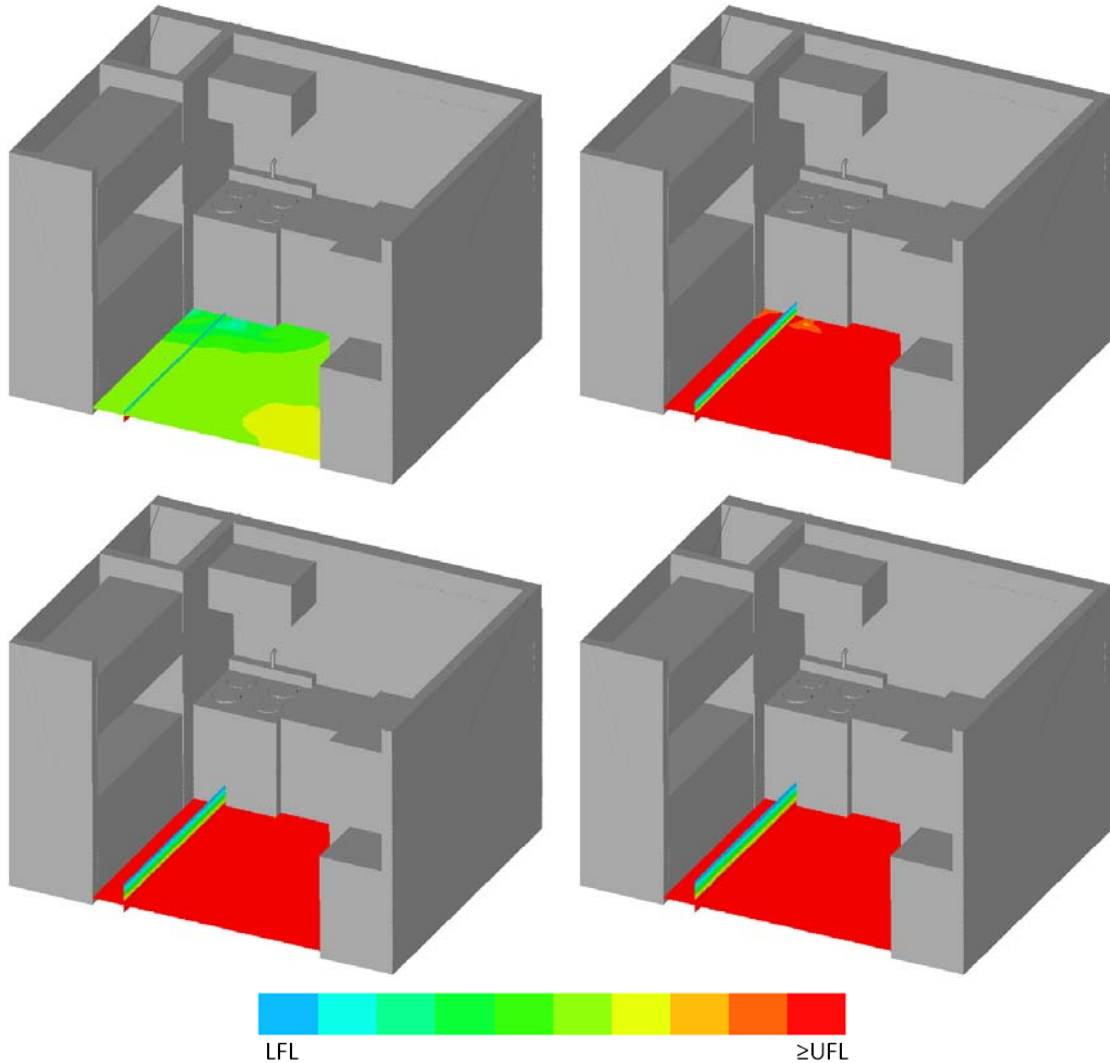
The impinging jet release scenario (propane leak from a 3/8-inch diameter horizontal hole and impinging against a wall approximately 0.4 m away) is shown in Figure 5. The propane jet exits the hole horizontally with a velocity of approximately 9.6 m/s and impinges against a wall while still at high momentum. As a result of the impingement, part of the propane jet is turned upward toward the stove exhaust fan (which is assumed sealed) and forms a flammable plume in the space above the range. The rest of the jet is redirected horizontally and spreads above the range/countertop surfaces as well as to the ground. Similarly to the free jet scenario, significant mixing occurs in the ground-level propane cloud, which is relatively well mixed and grows rapidly in thickness. The main difference between the free and impinging jet scenarios is

observed in the gas layer above the countertop surfaces, which is more stratified (and partially above the UFL) in the latter case.



**Figure 5. Propane cloud concentration from impinging jet leak, after: 5 minutes (top-left); 15 minutes (top-right); 30 minutes (bottom-left); and 60 minutes (bottom-right).**

The ground-level diffuse release – which could be representative, for example, of a propane leak preferentially flowing down in the narrow gap between the range and the back wall with less air entrainment, or due to a leak inside the cabinet flowing slowly out the front – is shown in Figure 6. In this case, the low-momentum release spreads at ground level, forming a thin and stratified layer. As the leak continues, most of the propane layer becomes rich (i.e., above the UFL) so that only a small region at the interface between the gas and the air is in the flammable range. As Figure 6 shows, even after one hour the gas cloud remains highly stratified and low to the ground, clearly limiting the location of viable ignition sources and the explosion potential.



**Figure 6. Propane cloud concentration from ground-level diffuse leak, after: 5 minutes (top-left); 15 minutes (top-right); 30 minutes (bottom-left); and 60 minutes (bottom-right).**

For any given flammable leak scenario, two factors are critical to reconciling the forensic evidence:

1. Where (and after how long) the cloud was ignited. As Figures 3 to 6 showed, the flammable cloud reached different areas at different times, depending on the characteristics of the leak. In some cases, the dispersion of the flammable cloud within the space may not be entirely consistent with the assumptions of simplified models (for example, gravity-induced sloshing is often observed from elevated diffuse leaks, and the amplitude of these oscillations is difficult to predict on the basis of zone models). These dynamic effects could, in some cases, have a significant impact on which ignition sources may or may not have ignited the cloud.
2. The size of the flammable volume available at the time of ignition. Once the gas cloud is ignited, the flame front will propagate rapidly (in a matter of a few seconds) throughout the space; therefore, only the portions of the gas cloud within the flammable range will contribute to the flame front propagation and to the overpressure. To a great extent, the intensity of a partially confined vapor cloud explosion is proportional to the size of the flammable portion of the ignited cloud (other parameters, such as congestion and location

of ignition being the same). Figure 7 shows the flammable volume for the four scenarios described earlier: even though the four scenarios were assumed to have the same gas release rate, the fraction of gas within the flammable range is significantly different, especially when comparing high-momentum versus diffuse scenarios. By ignoring the effect of leak momentum on cloud mixing, therefore, an investigator might draw incorrect estimates of the amount of fuel within its flammability limits that should have leaked into the space. Furthermore, another important parameter that is typically evaluated is the amount of fuel near stoichiometric or ideal concentrations, as this will have a direct effect on the outcome of an explosion.

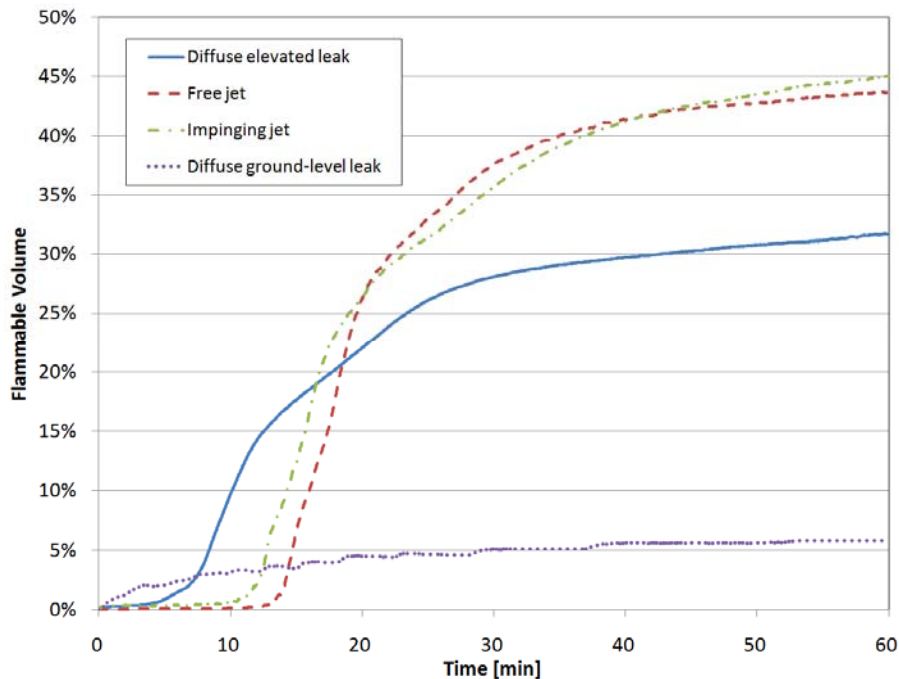


Figure 7. Flammable volumes for the four propane leak scenarios.

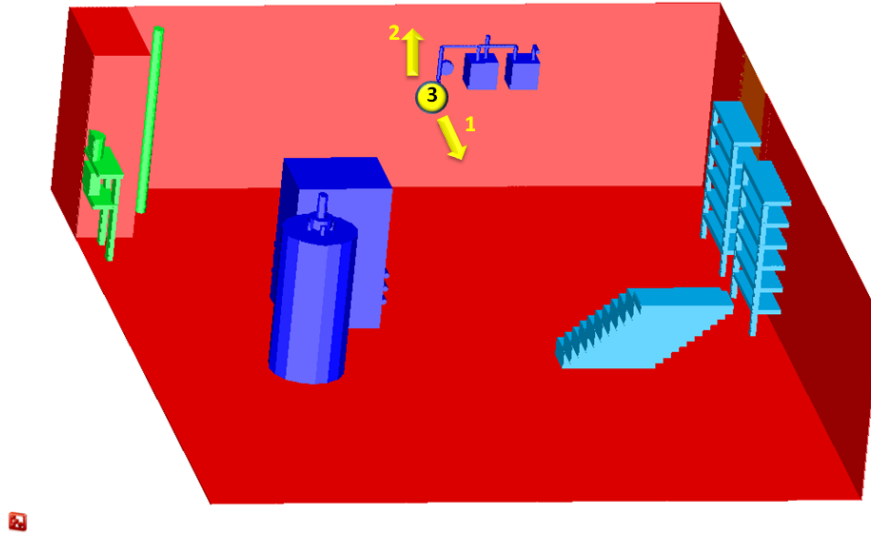
### CASE STUDY: NATURAL GAS LEAK IN A HOUSE BASEMENT

Another example of the effect of leak direction, this time for a positively buoyant gas leak (natural gas) is provided by the following: a high-pressure (approximately 60 psig) natural gas leak occurred in the basement of a multilevel home and, after continuing undetected for an unspecified amount of time, found an ignition source resulting in a deflagration that caused severe damage to the residence. Given the damage from the explosion, the inspection of the gas supply system revealed several potential leaks that had to be evaluated in order to determine which one (or more than one) might have led to a sequence of events consistent with the witness testimony and the forensic evidence gathered from the scene.

For the purpose of this paper, a reduced version of the leak investigation is provided. The following three natural gas leak scenarios were considered, as depicted in Figure 8:

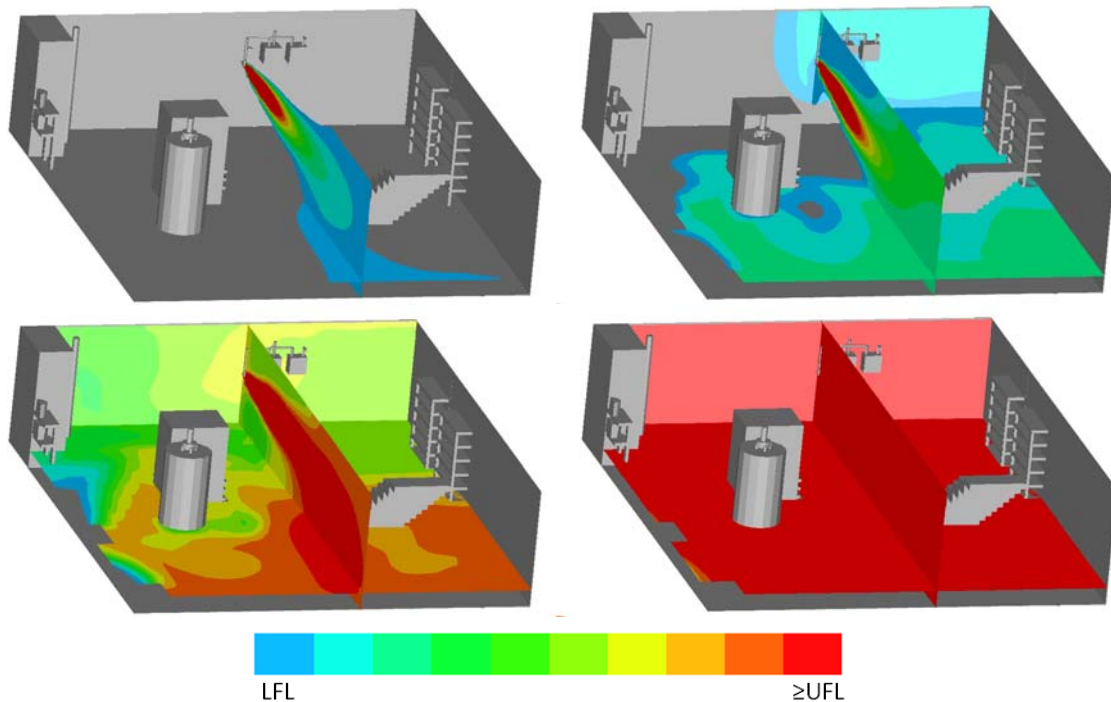
1. Free jet: a 0.38 kg/s (0.57 m<sup>3</sup>/s) leak from a 1-inch diameter hole directed horizontally and away from the wall;
2. Impinging jet: a 0.26 kg/s (0.39 m<sup>3</sup>/s) leak from a 3/4-inch diameter hole directed vertically and impinging against the basement ceiling;
3. Elevated diffuse release: a 0.38 kg/s low-momentum leak from the same location as scenario 1.

All leaks were assumed to last for 60 seconds, and initial conditions in the basement were quiescent air and 20°C in all scenarios. Air and gas could flow in/out of the basement through an opening at the top of the stairs, as well as through cracks along the perimeter of the basement ceiling.



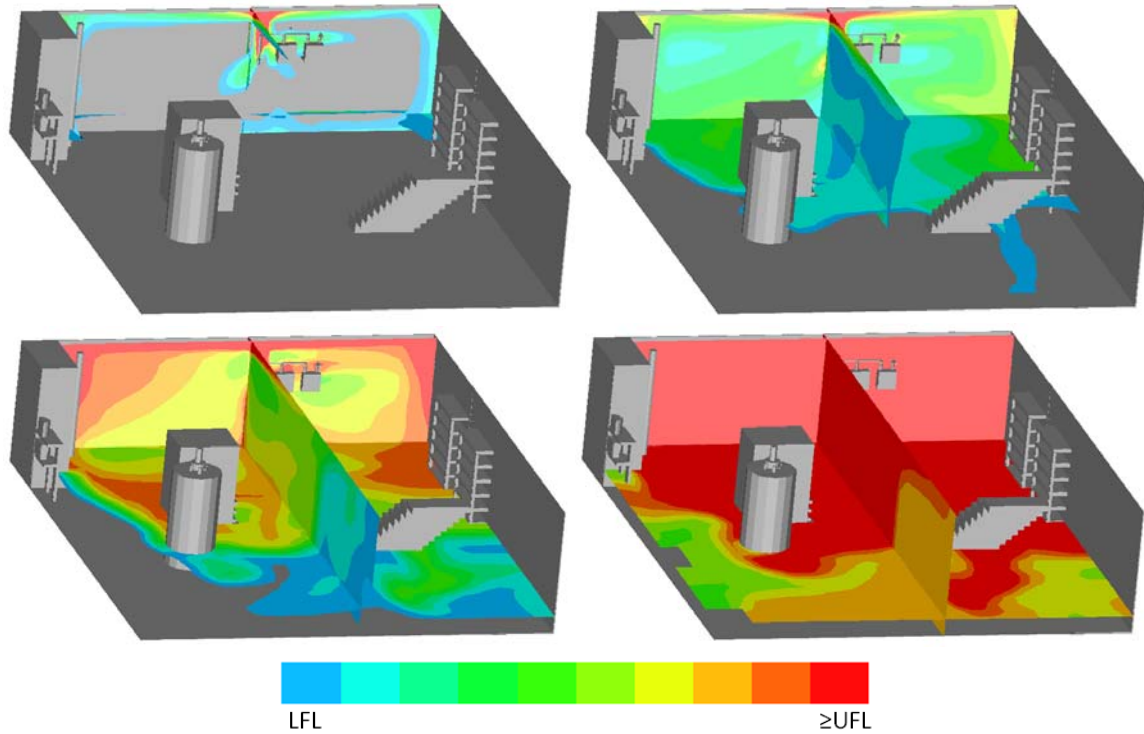
**Figure 8. Basement layout and natural gas leak scenarios.**

The free jet scenario sequence is shown in Figure 9. As for the case of propane discussed earlier, the jet-induced mixing forms a well-mixed flammable cloud over much of the basement. Due to the large leak rate in this scenario, after approximately 60 seconds the entire basement volume appears filled with a gas mixture at or above the UFL (15 mol% for methane).



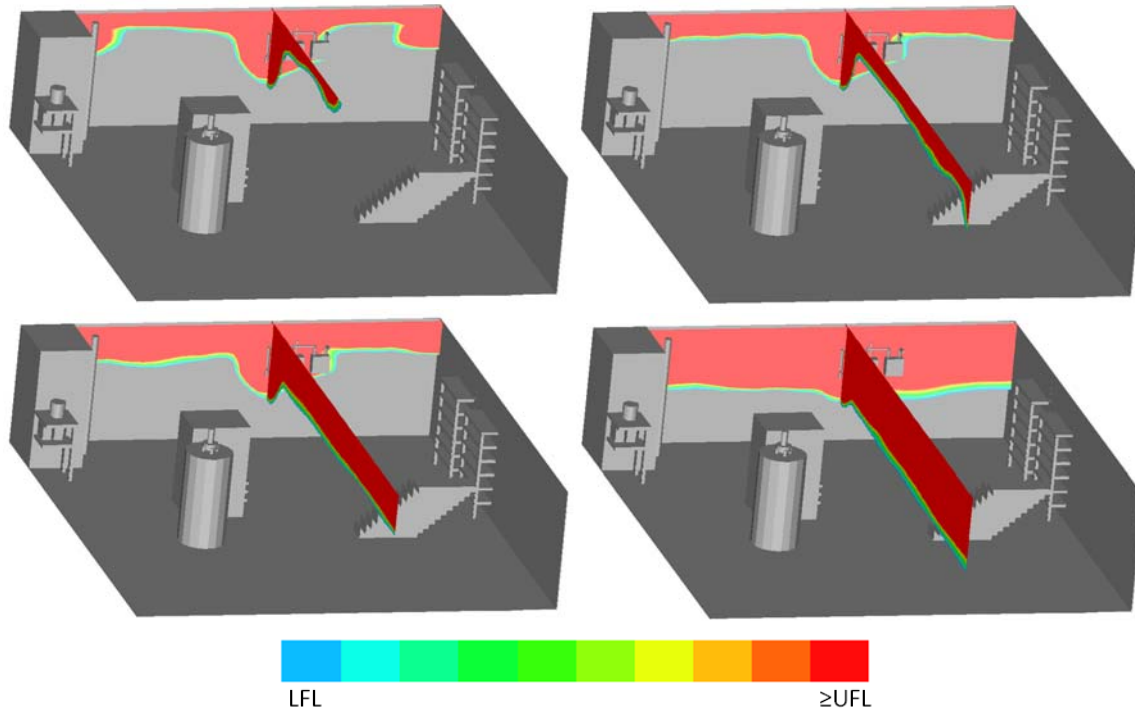
**Figure 9. Natural gas cloud concentration from the free jet, after: 5 seconds (top-left); 15 seconds (top-right); 30 seconds (bottom-left); and 60 seconds (bottom-right).**

The vertical natural gas jet impinging on the ceiling shows a very different evolution from the free jet. As shown in Figure 10, the impingement causes the jet to spread away from the stagnation point; due to the high momentum of the jet, the gas plume mixes with air and spreads to fill the volume surrounding the leak (see top-right image) – in apparent contradiction with common-sense expectations of the behavior of positively buoyant gases. Due to the presence of perimeter gaps in the basement ceiling and to the vertical momentum of the jet, a higher fraction of the gas release escapes the basement, so that after 60 seconds more than half of the basement remains in the flammable range.



**Figure 10. Natural gas cloud concentration from the impinging jet leak, after: 5 seconds (top-left); 15 seconds (top-right); 30 seconds (bottom-left); and 60 seconds (bottom-right).**

The low-momentum release is shown in Figure 11. In this case, the gas cloud rises towards the ceiling and stratifies, so that only a thin layer at the interface between the gas and the air is within the flammable range. As the leak progresses, the thickness of the gas cloud increases but the flammable volume remains approximately the same.



**Figure 11. Natural gas cloud concentration from low-momentum leak, after: 5 seconds (top-left); 15 seconds (top-right); 30 seconds (bottom-left); and 60 seconds (bottom-right).**

## CONCLUSIONS

This paper demonstrated how the use of a CFD model (FLACS) can provide detailed information on the dynamic behavior of a flammable gas cloud from an indoor leak. The results of the CFD simulations can be used to evaluate potential accident scenario for consistency with available forensic evidence, as required by the scientific method for fire and explosion investigations. The use of CFD-based numerical simulations allows the investigator to compare numerous scenarios and to perform sensitivity studies with respect to critical parameters in an efficient, cost-effective and safe manner.

While other tools, such as mathematical correlations or zone models, are often used to test origin and cause hypotheses, a three-dimensional CFD simulation can provide additional details on the dynamics of the flammable gas cloud that cannot be captured by a simplified model. In some cases, such as those described in this paper, small details in the release size or orientation can have a significant impact on the growth of the cloud and, consequently, on the location of viable ignition sources.

## ABOUT THE AUTHORS

Dr. Filippo Gavelli is the Head of Dispersion Consulting at GexCon US, and a Certified Fire and Explosion Investigator. He specializes in the analysis of heat transfer and fluid flow phenomena. He has over 15 years of experience with CFD modeling, which he applies to modeling the atmospheric dispersion of hazardous gaseous releases, as well as to the propagation of fires and explosions, utilizing GexCon's own CFD model, FLACS. GexCon specializes in explosion safety and develops the world-leading FLACS software, licensed to nearly 100 companies worldwide.

Dr. Scott Davis is the President at GexCon US. He specializes in mechanical engineering, and the engineering analysis and testing of combustion, thermal, and fluid processes. Dr. Davis is responsible for fire and explosion related consulting activities at GexCon, applying his expertise to the investigation,

prevention, and risk assessment of fires, gas and dust explosions, thermal runaway incidents and dispersion hazards such as flammable vapors and carbon monoxide exposures.

Olav R Hansen has been with GexCon (Norway) since 1993. GexCon specializes in gas explosion safety and develops and sells the world-leading FLACS software, licensed to nearly 100 companies around the world. Olav is currently the Product Director of GexCon. Formerly, he served as GexCon US' President and R&D Director of FLACS development and sales. Hansen is author or co-author of numerous papers within dispersion/explosion consequence modeling.

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