GAS RELEASE AND DISPERSION CFD MODULE FOR PREDICTING TRANSIENT FLAMMABLE AND POLLUTING GAS CLOUDS

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Introduction. In many industries, there are serious safety concerns related to the use of flammable gases in indoor and outdoor environments. It is important to develop reliable methods of analyses of flammable gas release and dispersion (GRAD) in real-life complex geometry cases. Computational fluid dynamics (CFD) is considered as one of the promising cost-effective approaches in such analyses**.** Over the last 6 years, the authors have been collaborating in CFD modeling of GRAD processes. As a result, the advanced robust CFD models have been developed, tested, validated and applied to the modeling of various industrial real-life indoor and outdoor flammable gas (hydrogen, methane, etc.) release scenarios with complex geometries. The user-friendly GRAD CFD modeling tool has been designed as a customized module based on PHOENICS. Advanced CFD models include the following: the dynamic boundary conditions, describing the transient gas release from a pressurized vessel, the calibrated outlet boundary conditions, the real gas law properties applied at high-pressure releases, the special output features and the local adaptive grid refinement (LAGR) tools. The predictions of transient 3D distributions of flammable gas concentrations have been validated using the comparisons with available experimental data. The validation matrix contains the enclosed and non-enclosed geometries, the subsonic and sonic release flow rates and the releases of various gases, e.g. hydrogen, helium, methane, etc. GRAD CFD module is recommended for safety and environmental protection analyses. It has been extensively applied to the hydrogen safety assessments including the analyses of hydrogen releases from pressure relief devices and the determination of clearance distances for venting of hydrogen storages. In particular, the dynamic behaviors of flammable gas clouds (with the gas concentrations between the lower flammability level (LFL) and the upper flammability level (UFL)) are accurately predicted with this module, which could be considered as a cost effective and reliable modeling tool for environmental assessments and design optimizations of combustion devices. The review paper[1] details the module features and provides currently available testing, validation and application cases relevant to the predictions of flammable gas dispersion scenarios. Below is a brief summary of this paper.

1. GRAD CFD module capabilities. GRAD CFD modeling tool has been designed as a customized module based on PHOENICS. One of the key features of PHOENICS is its easy programmability: it enables a user to add user-defined sub-models without a direct use of FORTRAN. This feature was used to incorporate the non-standard advanced GRAD sub-models, which include the following features: the dynamic boundary conditions, describing the transient gas release from a pressurized vessel; the calibrated outlet boundary conditions; the real gas law properties applied at high-pressure releases; the advanced turbulence models; the adaptive grid refinement tools; and the special output features.

1.1. Dynamic Boundary Conditions. In general, the transient (dynamic) boundary conditions should be applied at the flammable gas release location in order to properly describe the released gas mass flow rate, which depends on time. Depending on the pressure in the gas storage tank, the regime of release could be subsonic or sonic (choked). Assuming the ideal gas law equation of state and a critical temperature at the leak orifice and solving the first-order ordinary differential equation for density, $\rho(t)$, the transient mass flow rate at the sonic regime of release could be approximated as

$$\dot{m}(t) = -V\frac{d\rho}{dt} = \rho(t)u(t)A \approx \dot{m}_0 e^{-\frac{C_d A}{V}t\sqrt{\gamma(\frac{2}{\gamma+1})^{\frac{\gamma+1}{\gamma-1}}RT}},$$

$$\dot{m}_0 = C_d A\sqrt{\rho_0 P_0 \gamma(\frac{2}{\gamma+1})^{\frac{\gamma+1}{\gamma-1}}} \quad (1)$$

where u(t) is the flammable gas velocity at the leak orifice; V is the tank volume; $\dot{m}_0$, ρ_0 and P_0 are the flammable gas mass flow rate, the gas density in the tank and the gas pressure in the tank, respectively, at t=0; A is the leak orifice cross-sectional area; C_d is the discharge coefficient; and γ is the ratio of specific heats for flammable gas: $\gamma = C_P / C_V$, with C_P and C_V being the specific heat at constant pressure and constant volume, respectively. It should be noted that the choked release lasts until the ratio of the pressure in the tank over the ambient pressure, namely, P_0 / P_{atm} is greater than or equal to $(\frac{\gamma+1}{2})^{\frac{\gamma}{\gamma-1}}$ (it is about 1.90 for hydrogen).

1.2. Real Gas Law Properties. Under high pressure, flammable gases display gas properties different from the ideal gas law predictions. For example, at ambient temperature of 293.15˚K and a pressure of 400 bars, the hydrogen density is about 25% lower than that predicted by the ideal gas law. In order to account for real gas law behavior, the GRAD CFD module was provided with additional sub-models. In particular, for hydrogen release and dispersion modeling the Abel-Nobel equation of state (AN-EOS) was used to calculate the hydrogen compressibility, z_{H_2}, in terms of empirical hydrogen co-density, d_{H2} :

$$z_{H_2} = \frac{P}{\rho_{H_2} R_{H_2} T} = (1 - \frac{\rho_{H_2}}{d_{H_2}})^{-1}, \qquad (2)$$

where ρ_{H_2} , P, T and R_{H2} are the compressed hydrogen density, pressure, temperature and gas constant, respectively. It should be noted that the hydrogen compressibility, z_{H_2}, is equal to 1 for the ideal gas law. The hydrogen gas constant, R_{H2}, is 4124 J/(kgK). The hydrogen co-density, d_{H2}, is about 0.0645 mol/cm^3, or 129 kg/m^3. Equation (2) can be simplified as:

$$z_{H_2} = 1 + \frac{P}{d_{H_2} R_{H_2} T} \qquad (3)$$

The AN-EOS accounts for the finite volume occupied by the gas molecules, but it neglects the effects of intermolecular attraction or cohesion forces. It accurately predicts the high-pressure hydrogen density behavior[6].

1.3. Turbulence Model Settings. The turbulence models tested for GRAD modeling cases were as follows: LVEL model, k-ε model, k-ε RNG model and k-ε MMK model. It was found[1-8] that the LVEL model performs better in releases of flammable gas in congested spaces (indoor environment containing the solid blockages) and the k-ε RNG model performs better for jet releases in open space.

1.4. Local Adaptive Grid Refinement (LAGR). LAGR techniques are needed in GRAD CFD modeling in order to accurately capture the flammable cloud behaviors near the release location and in the locations with significant gradients of flammable gas concentration while considering large domains of practical interest. This refinement should be based on the local features of flammable gas mass concentration as a key unknown variable. The iterative technique of LAGR was developed, implemented into PHOENICS software, tested and validated for the two validation cases, namely, the hydrogen release within a hallway, and the helium release within a garage with a car (see picture below). The results of LAGR modeling were more accurate than the fixed grid solutions obtained with the standard grid refinement tools. However, additional development work and testing are needed in order to use LAGR on regular basis for GRAD modeling.

1.5. Special Output Features. The dynamics and extents of flammable gas cloud, containing the gas volume concentrations between LFL and UFL, are of major interest in any GRAD modeling. The total volume of space occupied by this cloud and the total mass of flammable gas in the cloud are listed as the special output features. GRAD CFD module calculates these special output quantities as functions of time based on the transient 3D distributions of gas concentrations and gas mixture density.

2. Validation work. Extensive GRAD CFD module validation work has been conducted over the last 6 years. Table 1 shows some validation cases.

Table 1. GRAD CFD module validation scenarios

Case No.	Case name	Description of experiment				CFD Model	Data source reference
		Domain	Leak direction	Leak type	Experimental data		
1	Helium jet	Open	Vertical	Subsonic, helium release	Steady-state, velocities, concentrations and turbulence intensities	Incompres. steady-state	Reference[11]
2	H_2 jet		Horizontal	Subsonic, H_2 release	Transient, concentrations	Incompress. transient	Reference[13]
3	INERIS Jet			Choked, H_2 release	Steady-state, concentrations	Compres. steady-state	Reference[14]
4	Hallway End	Semi-enclosed	Vertical	Subsonic, H_2 release	Transient, concentrations	Incompres. transient and steady-state	Reference[9]
5	Hallway middle			Subsonic, helium release	Transient, concentrations		
6	Garage with a car			Subsonic, H_2 and helium releases	Transient, concentrations		Reference[10]
7	H_2 vessel	Enclosed		Subsonic, H_2 release and dispersion	Transient, concentrations during dispersion	Incompres. transient	Reference[15]

2.1 Subsonic helium release in a garage with a car. One of the validation studies was conducted using the experimental and numerical data published by Dr. M.R. Swain et al.[10] on the helium subsonic release in a garage with a car. Figure 1 shows the geometry of the case considered. The green blocks mark the locations of four helium sensors in the domain.

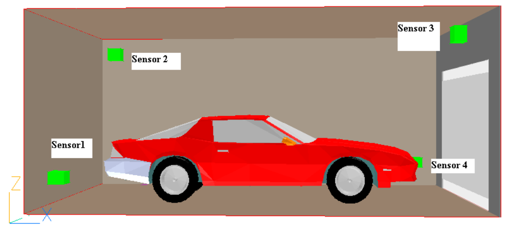

Figure 1. Geometry and sensors for subsonic helium release in a garage

Table 2 shows that LAGR helps reduce the predicted concentrations at the locations of Sensor 1 and Sensor 4 and make them closer to experimental values. The predicted results are in accord with the CFD simulations reported by Swain.

Table 2. Steady-state helium concentrations (LVEL turbulence model)

Simulations	Sensor 1	Sensor 2	Sensor 3	Sensor 4
Swain's CFD results	0.5%	2.55%	2.55%	1.0%
Initial coarse grid, 32×16×16	1.92%	2.53%	2.52%	1.94%
Adaptive refined, 39×26×24	0.98%	2.66%	2.62%	1.08%
Adaptive refined, 58×26×27	0.79%	2.70%	2.67%	1.01%

Conclusion

CFD modeling of flammable gas clouds could be considered as a cost effective and reliable tool for environmental assessments and design optimizations of combustion devices. In particular, the GRAD CFD module, which has been developed and validated, is recommended for safety and environmental protection analyses. Transient behaviors of flammable and polluting gas clouds can be accurately predicted with this modeling tool.

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