

GUIDANCE NOTES ON

GAS DISPERSION STUDIES OF GAS FUELED VESSELS

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American Bureau of Shipping Incorporated by Act of Legislature of the State of New York 1862

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Foreword

These Guidance Notes provide general information and guidelines on simulating dispersion of vented gas from a pressure relief valve (PRV) using Computational Fluid Dynamics (CFD) analysis.

International, regional, and local legislation is driving the development of alternative fuels to reduce exhaust emissions from ships. New technologies are primarily aimed at satisfying the IMO MARPOL Annex VI Regulations 13 and 14 requirements for nitrogen oxide (NO_x) emissions from diesel engines and sulfur oxide (SO_x) emissions from all fuel-burning equipment on board. One solution to the compliance with the SO_x emission limits of the MARPOL Annex VI Regulation 14, and potentially (for certain engine types) the NO_x limits of Regulation 13, is to use natural gas as a fuel or other low flashpoint fuels which are inherently low in sulfur.

The adoption of the International Code of Safety for Ships Using Gases or Other Low-Flashpoint Fuels (IGF Code) by the IMO Resolution MSC.391(95)(3) in June 2015 provided the IMO regulatory safety requirements and framework for the use of natural gas and other low flashpoint fuels on all ship types.

The applicable sections of the ABS *Rules for Building and Classing Marine Vessels (Marine Vessel Rules)* (5C-13-6/7) align with the IGF Code and require that vent exits of pressure relief systems for vessels using gases or other low-flashpoint fuels be located not less than one-third of the vessel breadth or 6 m (19.7 ft) (whichever is greater) above the weather deck; 6 m (19.7 ft) above working area and walkways; and at least 10 m (32.8 ft) away from air intakes, air outlets or openings to accommodation, service and control spaces, or other non-hazardous areas.

Because of the size limits, it may be impractical for some small vessels to meet these requirements. The ABS Rules recognize this and allow alternative arrangements to be accepted on a case-by-case basis. An appropriate risk assessment based on vessel-specific gas dispersion analysis is required.

These Guidance Notes were developed on the basis of industry experience mostly for vessels less than 60 m (197 ft) in length but may be applicable to larger vessels with additional considerations.

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CONTENTS				
SECTION 1	Intro	duction		1
	1	Gene	ral	1
	3	Indus	try Practices for Venting Systems	1
	5	ABS I	Rules and IMO Regulations for Vent Exit Location	1
	7	Overv	view of the Guidance Notes	2
	9	Defini	tions and Abbreviations	2
		9.1	Terms and Definitions	2
		9.3	Abbreviations	2
SECTION 2	Gen	eral Gui	delines for CFD Modeling of Gas Dispersion	4
	1	Mode	I Setup	4
		1.1	Computational Domain	4
		1.3	Boundary Conditions	4
		1.5	Computational Mesh	5
		1.7	Initial Conditions	5
	3	Mode	I Validation	6
	5	Mode	I Scenarios and Conditions	6
		5.1	Recommended Scenarios	6
		5.3	Characteristics of Gas Release	6
		5.5	Ambient Wind Condition	7
		5.7	Ambient Temperature	7
	7	Repo	rting of Simulation Results	7
APPENDIX 1	Case	e Study	of Gas Dispersion Simulation	8
	1	Case	Description	8
	3	CFD I	Model Description	8
	5	Mode	I Setup and Results	9
		5.1	Computational Domain and Boundary Conditions	9
		5.3	Grid Convergence Test	10
		5.5	Results	11
	7	Sensi	tivity Study	14
	9	Sumn	nary	21

	TABLE 1	Input Parameters for the Gas Dispersion Study Case	8
	TABLE 2	Summary of Boundary Conditions	9
	TABLE 3	Summary of Test Cases for Sensitivity Study	15
	FIGURE 1	Schematic Diagram of Computational Domain	9
	FIGURE 2	CFD Grids and Simulated % LEL Colormaps at Central Vertical Plane	10
	FIGURE 3	50% LEL for Coarse, Medium, and Fine Grids at Central Vertical Plane (Left) and Cross Section at 10 m Downwind from the Vent Exit (Right)	11
	FIGURE 4	U-velocity (m/s) and % LEL at Central Vertical Plane for the 6 m/s Wind Case (Steady State)	11
	FIGURE 5	% LEL at Central Vertical Plane during PRV Closing for the 6 m/s Wind Case	12
	FIGURE 6	U-velocity (m/s) and % LEL at Central Vertical Plane for the 1 m/s Wind Case (Steady State)	13
	FIGURE 7	% LEL at Central Vertical Plane during PRV Closing for the 1 m/s Wind Case	14
	FIGURE 8	Sensitivity Test Results on the Maximum Downwind Distance ($L_{50\% LEL}$) and the Maximum Height ($H_{50\% LEL}$) of the 50% LEL Contour	16
	FIGURE 9	50% LEL Contours for Different Gas Release Velocities for the 6 m/s Wind Case and the 1 m/s Wind Case	17
	FIGURE 10	50% LEL Contours for Different Release Gas Temperatures for the 6 m/s Wind Case and the 1 m/s Wind Case	; 18
	FIGURE 11	50% LEL Contours for Different Vent Orientations for the 6 m/s Wind Case	19
	FIGURE 12	50% LEL Contours for Different Ambient Temperatures for the 6 m/s Wind Case	19
	FIGURE 13	50% LEL Contours for Different Turbulent Schmidt numbers for the 6 m/s Wind Case	; 19
	FIGURE 14	Simulated Colormaps of % LEL at Central Vertical Plane for Different PRV Closing Times When the Valve is 50% and Fully Closed	20
	FIGURE 15	Locations of Maximum Distance of Gas Cloud 50% LEL during Closing	21
APPENDIX 2	Example of	Vent Exit Optimization	. 22
	1 Case	Description	22
	3 Mode	el Setup	22
	5 Resu	ılts	23
	7 Sum	mary	25
	TABLE 1	Simulated Maximum Speed in the Entire Domain (Unit: m/s)	23
	TABLE 2	Summary of Simulated Vertical Velocity at <i>z</i> = 10 m (Unit: m/s)	24
	TABLE 3	Summary of Simulated Drag Force on the Cone (Unit: N)	24

FIGURE 1		Original Vent Exit Design (Flat Lid) and Cone-shaped Vent Exit Designs with Various Cone Angles (A1~A6) and Positions (P1~P5)	22
	FIGURE 2	Computational Domain and Mesh	23
	FIGURE 3	Simulated Velocity Magnitude for the Lid Design and Cone Design (P3A2)	24
APPENDIX 3	Examples	of Validation Data	. 26
	1 Intro	oduction	26
	3 Rol	Ind Jet of Methane	26
	3.1	Case Description	26
	3.3	Model Setup	27
	3.5	Results	28
	5 Var	iable-density Axisymmetric Jets	29
	5.1	Case Description	29
	5.3	Model Setup	30
	5.5	Results	31
	TABLE 1	Parameters in the Methane Jet Case	27
	TABLE 2	Parameters of the Varied-density Axisymmetric Jets	29
	FIGURE 1	Schematic Diagram of a Supercritical Jet Release	26
	FIGURE 2	CFD Meshes of Horizontal Cross Section at $z = 0$ m	27
	FIGURE 3	Simulated and Measured Velocity and Molar Fraction of CH₄ along the Centerline	28
	FIGURE 4	Colormaps of Simulated Velocity and Molar Fraction of CH4	28
	FIGURE 5	Schematic Diagram of the Variable Density Jet Simulations	29
	FIGURE 6	Computational Domain and Mesh for the Variable Density Jets	30
	FIGURE 7	Simulated Centerline Velocity and Mass Concentration of Helium Jet	31
	FIGURE 8	Radial Profiles of Simulated Velocity and Mass Concentration of Helium Jet	31
	FIGURE 10	Simulated Centerline Velocity and Mass Concentration of CO ₂ Jet	32
APPENDIX 4	Basic Pror	perties of Methane	33
	TABLE 1	Basic Properties of Methane (CH ₄)	
	.,		
	FIGURE 1	Buoyancy of Methane Gas-Air Mixture	33
	FIGURE 2	Neutral Buoyancy of Methane Gas-Air Mixture at Different Ambient Temperatures	34

APPENDIX 5	Gas Dispers	sion Exclusion Zone Graph	. 35
	TABLE 1	Gas Release Parameters and Ambient Condition	.35
	FIGURE 1	Gas Dispersion Exclusion Zone at Ambient Temperature of –25°C	36
	FIGURE 2	Gas Dispersion Exclusion Zone at Ambient Temperature of 30°C	36
APPENDIX 6	References		. 37



SECTION 1 Introduction

1 General

For vessels using gases or other low-flashpoint fuels, the ABS *Rules for Building and Classing Marine Vessels (Marine Vessel Rules)* (5C-13-6/7.2) require the vent exit of pressure relief systems to be located not less than one-third of the vessel breadth or 6 m (19.7 ft), whichever is greater, above the weather deck; 6 m (19.7 ft) above working area and walkways; and at least 10 m (32.8 ft) away from air intakes, air outlets or openings to accommodation, service and control spaces, engine combustion air intakes (5C-13-10/3.1.11 of the *Marine Vessel Rules*), or other non-hazardous areas.

Because of their size limits, it may be impractical for some small vessels to meet these requirements. The ABS Rules recognize this and allow alternative arrangements to be accepted on a case-by-case basis. An appropriate risk assessment based on a vessel-specific gas dispersion analysis is required in accordance with recognized standards (e.g., IEC-60079-10-1).

Computational Fluid Dynamics (CFD) has been widely recognized as a useful tool for assessing various engineering applications. In comparison to other approaches such as empirical correlations models (Chen & Rodi, 1980) and integral models (Lee & Chu, 2003), CFD is an advanced modeling technology which solves the conservation equations of mass, momentum, gas species, energy, and turbulence and provides detailed information on the gas cloud in both near and far fields. A summary of the capabilities and limitations of these modeling approaches can be found in Ivings et al. (2007).

These Guidance Notes provide the general information and guidelines for carrying out a gas dispersion study using CFD. These Guidance Notes were developed on the basis of industry experiences mostly for vessels less than 60 m (197 ft) in length and are not intended to address all aspects of gas dispersion CFD analysis. Application to larger vessels may need additional considerations.

3 Industry Practices for Venting Systems

In accordance with prescribed regulations and requirements, the design of the venting systems connected to the pressure relief valves (PRVs) should consider the location of the vent exit, the discharge direction, and the prevention of water and snow ingression. Taking into account specific situations and arrangements, various vent exit arrangements as follows have been practically proposed and designed along with advanced analyses (e.g., gas dispersion study) to prove compliance with the intended requirements.

- Vertically upward venting with a vent height less than 6 m (19.7 ft) or near by non-certified safe equipment
- Venting with a direction different from vertically upward
- Ventilation with the tank vent outlet.

5 ABS Rules and IMO Regulations for Vent Exit Location

- ABS Rules for Building and Classing Marine Vessels, 5C-13-6/7.2
- ABS Rules for Building and Classing Marine Vessels, 5C-13-10/3.1.11
- International Code of Safety for Ships using Gases or other Low-Flashpoint Fuels (IGF Code), 6.7.2

7 Overview of the Guidance Notes

These Guidance Notes provide technical guidelines and sample calculations for the typical gas dispersion analysis for assessing an alternative vent exit arrangement.

Section 2 addresses the general guidelines for CFD model setup and choices of test conditions for gas dispersion simulations. Recommended reporting of simulation results is also specified.

To provide an example, Appendix 1 presents a typical case study. In addition, the sensitivity of the gas cloud to different parameters and ambient conditions are examined.

Appendix 2 contains an example of a vent design optimization study aiming to enhance the vent exit velocity, which was identified as one of the critical parameters to a gas cloud based on a sensitivity study.

Examples of model validation for gas dispersion and basic properties of methane are provided in Appendices 3 and 4, respectively.

Appendix 5 presents a sample exclusion zone graph developed based on CFD simulations of conservative scenarios. The graph can be used for pre-screening of a venting design before conducting a full design optimization.

9 Definitions and Abbreviations

9.1 Terms and Definitions

The following terms and definitions are used in these Guidance Notes.

Back Pressure. The pressure drop due to a resistance or force opposing the desired flow through a vent pipe.

Boiling Point. The temperature at which a liquid changes to vapor at the ambient pressure.

Exclusion Zone. The maximum distance from the gas release point to where the predicted mean gas concentration falls to half the Lower Explosive Limit (LEL).

Flashpoint. Lowest liquid temperature at which a liquid gives off vapors in a quantity that can form an ignitable vapor/air mixture.

Hazardous Area. An area where an explosive gas atmosphere is or may be expected to be present.

Upper Explosive Limit (HFL). The concentration of flammable gas in air above which an explosive gas atmosphere cannot be formed.

Lower Explosive Limit (LEL). The concentration of flammable gas in air below which an explosive gas atmosphere cannot be formed.

Non-Hazardous Area. An area where an explosive gas atmosphere is not expected to be present.

Normal Operation. The situation when the vessel is operating within its designed parameters.

Pressure Relief Valve (PRV). A valve used to control or limit the pressure in a fuel storage tank by releasing LNG gas to the atmosphere through a vent pipe.

Turbulence Intensity (TI). A measure of turbulence level defined as the root mean square of local velocity fluctuations relative to the mean velocity.

Turbulent Schmidt Number. The ratio between turbulent viscosity of flow and turbulent diffusivity of a gas specie.

9.3 Abbreviations

- ABL Atmospheric Boundary Layer
- CFD Computational Fluid Dynamics
- UEL Upper Explosive Limit
- LEL Lower Explosive Limit

- PRV Pressure Relief Valve
- TI Turbulence Intensity



SECTION 2 General Guidelines for CFD Modeling of Gas Dispersion

1 Model Setup

The guidelines presented here are intended to be general, and software-specific settings are not in the scope of these Guidance Notes.

1.1 Computational Domain

The dimensions of the computational domain depend on the extent of the gas cloud, the size of area to be studied, and the boundary conditions that will be applied.

The boundaries of the computational domain should be sufficiently far from the area of interest so as to avoid any adverse effects from the approximations of boundary conditions.

If the simulation is repeating a wind tunnel experiment for validation purposes, the domain size should be consistent with that of the wind tunnel experiment.

1.3 Boundary Conditions

Boundary conditions should be chosen to properly represent the surroundings that have been cut off by the computational domain. Improper selection of boundary conditions may lead to physically incorrect results.

Boundary conditions for all flow variables (i.e., velocities, pressure, and temperature), turbulence quantities (which depend on the turbulence model used), and gas concentration need to be specified at the boundaries.

If the simulation is repeating a wind tunnel experiment for validation purposes, the boundary conditions should be consistent with the wind tunnel conditions.

The boundary conditions for a cuboid computational domain commonly applied for gas dispersion modeling are described below.

1.3.1 Gas Inlet Boundary Conditions

At the gas inlet boundary, the gas release velocity, temperature, and gas composition are known and assigned directly. The local pressure condition is not user-specified but calculated by the CFD model.

Specification for turbulence quantities depends on the selection of turbulence model. For many engineering applications including gas dispersion, two-equation turbulence models are often used. As an example, if the k-epsilon turbulence model is used, the turbulence kinetic energy (k) and turbulence dissipation rate (ε) at the inlet boundaries may be estimated using the following formulae:

$$k \approx \frac{3}{2} (\overline{UI})^2 \quad \text{m}^2/\text{s}^2 (\text{ft}^2/\text{s}^2)$$
$$\varepsilon \approx C_\mu \frac{k^{3/2}}{L} \quad \text{m}^2/\text{s}^3 (\text{ft}^2/\text{s}^3)$$

where

 \overline{U} = mean flow velocity, in m/s (ft/s)

I =turbulence intensity, in %

- L =turbulence length scale, in m (ft)
- C_{μ} = turbulence model constant (= 0.09)

Typically, the turbulence intensity for a moderately turbulent flow is between 1% and 5%. Turbulence quantities may be estimated using an online tool found on *CFD Online* through the link *https://www.cfd-online.com/Tools/turbulence.php*.

1.3.2 Wind Inflow Boundary Conditions

At the wind inflow boundary, prescribed profiles of mean wind velocity and turbulence quantities are often applied based on the equilibrium atmospheric boundary layer (ABL) assumption (i.e., the production and dissipation rates of the kinetic energy of turbulence are equal to each other). The mean wind velocity is usually a logarithmic profile corresponding to a roughness length, (e.g., 0.0002 m (0.00066 ft) for open sea surfaces (*WMO-No. 8*) and the wind speed at the reference height. The prescribed profiles should not change until the location of gas release is reached. It is suggested to carry out a simulation in an empty domain with the exact same grid and boundary conditions before conducting a gas release simulation.

Ambient temperature should be specified explicitly on the wind inlet boundary.

Available data from nearby meteorological stations may be used to determine the ambient wind speed at the reference height and ambient temperature.

1.3.3 Wall Boundary Conditions

Wall boundary conditions can be applied on the surfaces of the hull and vent mast, sea/ground surface, or any solid walls in the simulation. At the wall boundary, the no-slip boundary condition is used for the velocities, which means the air has zero velocity relative to the boundary. Wall functions are often used for calculations of wall shear stress and turbulence quantities. All other variables are typically not user-specified but calculated based on the CFD solution.

1.3.4 Symmetric Boundary Conditions

Symmetric boundary conditions can be used at lateral boundaries when the wind direction is parallel to the boundaries. At the symmetric boundary, the normal velocity component is forced to be zero. Symmetric boundary should be sufficiently far from the gas release to avoid any artificial flow generated. All other variables are typically not user-specified but calculated based on the CFD solution.

1.3.5 Outflow Boundary Conditions

Outflow boundary conditions are used to model flow exit from the domain where the flow is fully developed. The outflow boundary should be far away enough from the gas release to avoid generation of any artificial flow. The outflow boundary condition may also be applied on the top and lateral boundaries that are located far away enough from the gas release.

1.5 Computational Mesh

The resolution of the computational mesh should be fine enough to capture the physical phenomena of interest. The necessary resolution should be determined by conducting a systematic grid convergence test.

1.7 Initial Conditions

The larger the computational domain and the smaller the wind speed, the greater the influence from the initial conditions.

For a steady-state solution, the solution is mainly affected by the boundary conditions. The simulation stops when the solution converges. Initializing the domain with a flow field that is close to the final solution will reduce the computational resources needed to reach the steady-state solution. In most cases, a good starting point is to initialize the domain with the wind inflow data.

For an unsteady solution, the initial condition affects the time development of the simulation and should be considered carefully. For example, the steady-state solution may be used as the initial condition to simulate a PRV closing. A time-step convergence test should be performed in conjunction with a gird convergence test before the CFD model can be used for application.

3 Model Validation

Model validation is a process to evaluate a model's performance by comparing the simulated results against experimental results. It should be noted that there are many factors, including both physical and numerical parameters, that can affect the gas dispersion results. Therefore, it is important to demonstrate that acceptable levels of uncertainty and error are provided in the CFD simulations.

Examples of model validation data are provided in Appendix 3.

5 Model Scenarios and Conditions

5.1 Recommended Scenarios

For the purpose of hazard assessment, the test conditions covering the worst-case scenarios should be evaluated, with consideration of the vessel's venting arrangements and operational conditions.

Prior to conducting a detailed gas dispersion study (quantitative risk assessment), qualitative risk assessment should be performed to identify hazardous scenarios associated with the proposed design as per 5C-13-4/2 of the *Marine Vessel Rules*. Risk assessment procedure and technique may refer to 5C-8-A7/3.7.1 of the *Marine Vessel Rules*.

5.3 Characteristics of Gas Release

The gas release condition is one of the key inputs for modeling gas dispersion. The expected gas release condition should be considered carefully, including the following:

- *i)* Vent exit diameter
- *ii) Vent Exit Location.* The actual elevation of the vent exit above the sea level should be considered in the simulation since the background wind and turbulence are varied at different elevations and affect the mixing of the released gas cloud.

If the vessel is included in the simulation, the location of the vent exit should be specified accordingly.

- *iii)* Gas release orientation
- *iv)* Gas Release Rate at the Vent Exit. The total mass flow rate should be considered in the case of using multiple PRVs or bypass valves.
- v) Closing Duration of the Relief Valve or the Designated Control Valve. PRVs open upon overpressurization in the storage tank. Depending on the valve types and configurations, the closing time of valves should be specifically defined and selected. Consideration should be given to the timedependent gas release rate during closing.

In the case of using bypass valves, a fast closing could be applied manually by the ship crew and should be considered accordingly.

vi) Gas Release Duration. During normal operating conditions, the duration of gas release is expected to be a relatively short period of time. However, to be conservative, it is recommended that the simulated duration of gas release is long enough for the gas cloud to reach its steady state, which means the gas cloud boundary (e.g., 50% LEL) is no longer changing with time.

The simulation of PRV closing period should follow after the gas cloud reaches its steady state. During the closing period, the gas cloud may start to descend due to the reduced initial momentum. Once the PRVs are fully closed, the simulation should continue to model the tailing of the gas cloud until the gas concentration is diluted below 50% LEL.

- *vii)* Gas Composition. Gas composition may depend on the composition of the LNG in the storage tank. Pure methane may be modeled if the gas data is not available. An example of methane properties is given in Appendix 4.
- *viii)* Gas Release Temperature. The gas release temperature at the vent exit may be set to the expected lowest gas vapor temperature in the storage tank with the assumption that there is no heat loss between the storage tank and the vent exit. It is noted that the liquid fraction in the gas release may be considered when the temperature is low enough.

5.5 Ambient Wind Condition

Ambient wind is a critical factor to gas dispersion and calls for careful consideration. Wind condition is closely related to the ambient turbulence. For example, the Pasquill stability table requires solar radiation and wind speed for estimating ambient turbulence level (Pasquill, 1961).

For ships operating in restricted areas or between specific ports, if weather data from nearby meteorological stations is available, a representative of the wind speed in the areas may be developed based on wind statistics for the assessment (refer to IEC 61400-1-11.3 and IEC 61400-3-6). In addition, a reduction factor considering the reference height applied for the weather stations should be applied (refer to IEC 60079-10-1:C.3.4).

If weather data is not available, low wind speed in a stable atmospheric condition is often considered the worst-case scenario and should be used. For selection of wind speed, refer to IEC 60079-10-1 Table C.1.

Wind directions toward non-hazardous areas should be considered as the worst-case scenarios.

5.7 Ambient Temperature

Ambient temperature is important to gas dispersion, especially in low wind conditions when the buoyancy force (i.e., due to the density difference between the gas cloud and ambient air) plays a more significant role than in high wind conditions.

When gas is released and mixed with ambient air, the density of the gas cloud varies with the gas fraction and the temperature of the mixture. The gas cloud is buoyant when its density is lighter than that of ambient air or is negatively buoyant otherwise. An example of the buoyancy regions for methane gas at different ambient temperatures is provided in Appendix 4.

For ships operating in restricted areas or between specific ports, a representative of the ambient temperature in the areas may be developed based on the weather statistics from a nearby meteorological station (refer to IEC 61400-1-11.5 and IEC 61400-3-6) for the assessment.

7 Reporting of Simulation Results

The report should contain the following information in detail:

- *i)* Basic information of the CFD model (e.g., methodology, assumptions, governing equations, turbulence model, boundary conditions, and ABL implementation).
- *ii)* Model validation (e.g., a comparison of the CFD results with appropriate experimental data or analytical formulations).
- *iii)* Model setup information (e.g., description of the venting arrangement and system, possible scenarios, characteristics of gas release, and ambient conditions).
- *iv)* Grid and time-step convergence test (e.g., comparison of results using different grid sizes or time steps.
- *v)* Graphical results:
 - *a)* Flow field
 - *b)* Colormap of % LEL
 - *c)* % LEL contour (e.g., 50% LEL)

The locations of the graphical output should include the vertical center plane of the gas cloud and any other locations of interest.

In the graphical output, sufficient labeling and legends should be provided. Potentially sensitive receptors (e.g., air intakes and air outlets) may be also indicated in the graphics.

The percentage of LEL to define the gas cloud as the acceptance criteria should be based on the risk assessment results.

- *vi)* Time histories of % LEL at locations of concern
- *vii)* The time for which the gas cloud (e.g., 50% LEL) persists after the release stops
- *viii)* Conclusions and recommendations



APPENDIX 1 Case Study of Gas Dispersion Simulation

1 Case Description

The study case is based on a vent system design of a dual fuel tugboat. The tugboat is approximately 32 m in length, and 12.5 m in width. The LNG vent mast is 6 m in height and located above the top of the wheel house. The vent exit is at the elevation of 18.7 m above the mean water surface. The gas release velocity is 66 m/s as estimated using IMO Resolution A.829(19).

An unsteady gas release is modeled to account for the PRV closing. In the simulation, the PRV is modeled fully opened until the solution reaches steady state, followed by a closing time lasting 20.8 s. The gas release velocity decreased linearly during the closing period. The corresponding release flow rate is calculated based on the vent opening area.

Two wind conditions are simulated, including 6 m/s (Pasquill stability Class D, which represents neutral conditions) and 1 m/s (Pasquill stability Class F, which represents very stable conditions). Other input parameters are listed in Appendix 1, Table 1.

Parameter	Symbol	Value
Vent diameter	D	0.24 m
Release gas component (molar fraction)	Y_i	93.41% CH4; 6.24% C ₂ H ₆ ; 0.3% N ₂ ; 0.05% C ₃ H ₈
Release velocity	U_j	66 m/s
Vent orientation	-	Upward
Release gas temperature	T_j	-161°C
PRV closing duration	T_c	20.8 s
Ambient temperature	T_a	30°C
Wind conditions	U_a	1 m/s; 6 m/s
Surface roughness	Z0	0.0002 m

TABLE 1Input Parameters for the Gas Dispersion Study Case

3 CFD Model Description

This case study is provided to demonstrate CFD modeling of gas dispersion. The model parameters presented here are case-specific.

5 Model Setup and Results

5.1 Computational Domain and Boundary Conditions

The computational domain for CFD simulations is constructed using an upstream wind inlet boundary, open boundaries (top, outlet, and sides), bottom, vent mast wall, and vent inlet. For the 6 m/s wind case, the dimensions of the domain are 170 m, 40 m, and 66 m in the x, y, and z axes, respectively. The vent mast is located at 20 m downstream from the wind inlet boundary and 20 m to each side boundaries. The bottom boundary is 6 m below the vent exit. For the 1 m/s wind case, the domain bottom is extended downward by 7.7 m (i.e., 13.7 m below the vent exit). Appendix 1, Figure 1 shows a schematic of the computational domain.

At the wind inlet boundary, the fully-developed profiles of the mean velocity, turbulence kinetic energy, and dissipation rate (ABL boundary conditions) are imposed. The ABL boundary conditions are also applied on the bottom boundary.

A non-slip wall boundary condition is used on the vent mast wall. On the top, side, and outlet boundaries, zero gradient is applied for all variables, except that the pressure on the top boundary is prescribed as the hydrostatic atmospheric pressure.

A prescribed gas release velocity and temperature are applied at the vent inlet boundary. All the variables of interest for the boundary conditions are summarized in Appendix 1, Table 2.



FIGURE 1 Schematic Diagram of Computational Domain

TABLE 2 Summary of Boundary Conditions

	U m/s	$p_{ ho gh} Pa$	Temperature K	Y_i	$k m^2/s^2$	ε m^2/s^3
Bottom	ABL	Zero-gradient	Zero-gradient	Zero-gradient	ABL	ABL
Inlet	$(0,0,U_j)$	Zero-gradient	T_j	Fixed-value	$I_{turb} = 0.01$	$L_{turb} = 0.01$
Outlet	Zero-gradient	Zero-gradient	Zero-gradient	Zero-gradient	Zero-gradient	Zero-gradient
Side	Zero-gradient	Zero-gradient	Zero-gradient	Zero-gradient	Zero-gradient	Zero-gradient
Тор	Zero-gradient	101,325	Zero-gradient	Zero-gradient	Zero-gradient	Zero-gradient
Wall	(0,0,0)	Zero-gradient	Zero-gradient	Zero-gradient	Wall function	Wall function
Wind inlet	ABL	Zero-gradient	Tamb	Fixed-value	ABL	ABL

5.3 Grid Convergence Test

A grid convergence test is first performed to investigate how the gas cloud could be affected by the grid size. The vent exit is represented by 64 cells (\sim 0.025 m). Three different grid resolutions, including coarse (1 m), medium (0.5 m), and fine (0.25 m) grid sizes, in the far field are tested (Appendix 1, Figure 2). It should be noted that the refinement region is on the lower part of the domain where the gas cloud is present, and the grid size at the vent exit remains the same. The total cell numbers for the coarse, medium, and fine grids are about 0.28, 1.2, and 7.7 million, respectively.

The convergence test conditions are based on the study case (see Appendix 1, Table 1). The wind speed is 6 m/s.

Appendix 1, Figure 2 also shows the distribution of the simulated % LEL. Appendix 1, Figure 3 displays the 50% LEL boundary on the central vertical plane and the cross section at 10 m downwind from the vent exit. The maximum downwind distance to the 50% LEL concentration from the vent exit is 47.0 m, 56.6 m, and 61.0 m based on the coarse, medium, and fine grids, respectively. The results show that the simulated contour of 50% LEL converges when the mesh is refined. With the consideration of both result accuracy and computational efficiency, the medium grid is chosen for the case study and sensitivity study, which are presented in the following sections.

FIGURE 2 CFD Grids and Simulated % LEL Colormaps at Central Vertical Plane





FIGURE 3 50% LEL for Coarse, Medium, and Fine Grids at Central Vertical Plane (Left) and Cross Section at 10 m Downwind from the Vent Exit (Right)



5.5 Results

Appendix 1, Figure 4 displays the colormaps of the U-velocity and % LEL at the central vertical plane at steady state for the 6 m/s wind case. The gas cloud traveled horizontally and remained around the same height. Appendix 1, Figure 5 shows the % LEL at different times during the closing of the PRV. The gas concentration decreased below 50% LEL about 1 s after the PRV was fully closed.

Similar plots for the 1 m/s wind case are also presented in Appendix 1, Figures 6 and 7. The gas concentration decreased below 50% LEL about 25 s after the PRV was fully closed.

The dispersion of the released gas behaved very differently in the 1 m/s wind case. The gas cloud initially had an upward trend due to the initial high momentum of the release. As the momentum decreased, the cloud had a downward trend due to its higher density than that of the ambient air.

FIGURE 4 U-velocity (m/s) and % LEL at Central Vertical Plane for the 6 m/s Wind Case (Steady State)



Note: The black solid curve is the 50% LEL Contour.



FIGURE 5 % LEL at Central Vertical Plane during PRV Closing for the 6 m/s Wind Case

Note: The black solid curve is the 50% LEL Contour.



FIGURE 6 U-velocity (m/s) and % LEL at Central Vertical Plane for the 1 m/s Wind Case (Steady State)

Note: The black solid curve is the 50% LEL Contour.



FIGURE 7 % LEL at Central Vertical Plane during PRV Closing for the 1 m/s Wind Case

Note: The black solid curve is the 50% LEL Contour.

7 Sensitivity Study

The case study described in the previous sections is used as the base case for the sensitivity study on different input parameters (i.e., gas release parameters, ambient conditions, and the turbulent Schmidt number for the gas release) (Appendix 1, Table 3). The purpose of the sensitivity study is to learn how sensitive the gas cloud is to the influence of those input parameters.

Parameter	Symbol	Values
Release velocity	U_j	20 m/s, 40 m/s, 60 m/s, 80 m/s, and 100 m/s
Release gas temperature	T_0	-161°C, -155°C, -150°C, -135°C, and -125°C
Vent Orientation*	ф	30°, 45°, 60°, 75°, and 90° (upward)
Ambient temperature	Ta	–25°C, 0°C, and 30°C
Turbulent Schmidt number	Sc_t	0.7, 0.8, and 1
PRV closing duration	T_c	20.8 s, 40 s, and 60 s

TABLE 3Summary of Test Cases for Sensitivity Study

* *Note:* ϕ is defined by the angle to the horizontal wind direction.

The gas cloud is evaluated by the maximum downwind distance to the 50% LEL concentration from the release point ($L_{50\% LEL}$) and its corresponding height above the mean sea level ($H_{50\% LEL}$), as shown in Appendix 1, Figure 8. For the 6 m/s wind case, the gas cloud is more sensitive to the gas release velocity and temperature than other parameters. A lower wind speed (i.e., 1 m/s) is also tested for both gas release velocity and temperature. The results indicate that $H_{50\% LEL}$ is affected more significantly than $L_{50\% LEL}$ in the low wind condition. The 50% LEL contours are presented in Appendix 1, Figures 9 to 13.

Three PRV closing times of 20.8 s, 40 s, and 60 s are also tested with the 6 m/s wind. Appendix 1, Figure 14 presents the colormaps of % LEL when the PRV is 50% closed and fully closed. The gas concentration decreased below 50% LEL within 1 s after the PRV was fully closed for all cases. Appendix 1, Figure 15 shows the locations of the maximum distance of 50% LEL. The results suggest that the closing time within 60 s does not affect the gas cloud significantly for this test condition.



FIGURE 8 Sensitivity Test Results on the Maximum Downwind Distance (*L*50%*LEL*) and the Maximum Height (*H*50%*LEL*) of the 50% LEL Contour

(e) Turbulent Schmidt number



FIGURE 9 50% LEL Contours for Different Gas Release Velocities for the 6 m/s Wind Case and the 1 m/s Wind Case

(b) 1 m/s wind





(a) 6 m/s wind



(b) 1 m/s wind

FIGURE 11 50% LEL Contours for Different Vent Orientations for the 6 m/s Wind Case



FIGURE 12 50% LEL Contours for Different Ambient Temperatures for the 6 m/s Wind Case



FIGURE 13 50% LEL Contours for Different Turbulent Schmidt numbers for the 6 m/s Wind Case



FIGURE 14 Simulated Colormaps of % LEL at Central Vertical Plane for Different PRV Closing Times When the Valve is 50% and Fully Closed



Note: The black solid curve is the 50% LEL Contour.



FIGURE 15 Locations of Maximum Distance of Gas Cloud 50% LEL during Closing

9 Summary

- *i)* A systematic grid convergence test was carried out to determine the appropriate grid resolution for the case study and sensitivity study. It was found that the gas cloud is sensitive to the grid resolution. The extent of the gas cloud is under-predicted when the grid is not fine enough.
- *ii)* The study case included two wind conditions (1 m/s and 6 m/s). The dispersion behavior of the released gas is very different between the two wind conditions. For the 6 m/s wind case, the gas cloud remained at about the same elevation of the vent exit. For the 1 m/s wind case, the gas cloud initially had an upward trend due to its initial high momentum, and then had a downward trend due to its relatively heavy density.
- *iii)* A sensitivity study on different gas release parameters, ambient conditions, and the turbulent Schmidt number was conducted. The gas cloud is characterized by the maximum downwind distance to the 50% LEL concentration from the release point and its corresponding height. The results suggest that the gas cloud is sensitive to gas release velocity and temperature.



APPENDIX 2 Example of Vent Exit Optimization

1 Case Description

CFD is utilized for evaluating a conventional vent exit design (flat lid) and optimizing a conceptual coneshape vent exit design by varying the angle and position of the cone for greater dilution of the gas cloud.

For the optimization, the decision variables include the vertical velocity at z = 10 m (10 m above the vent exit), the maximum speed, the drag force on the cone, and the back pressure. Constraints on the decision variables include:

- The maximum speed is less than the speed of sound
- Pressure drop is less than 30%

In this case, the gas enters the mast at a velocity of 26.37 m/s. The gas temperature is -161° C. Appendix 2, Figure 1 shows the original lid design and cone-shaped designs with various cone angles and positions (22 cone-shaped designs).

This example demonstrates the utility of CFD in assessing vent design and is not intended to be a complete design project.

FIGURE 1 Original Vent Exit Design (Flat Lid) and Cone-shaped Vent Exit Designs with Various Cone Angles (A1~A6) and Positions (P1~P5)



3 Model Setup

The dimensions of the computational domain are 20 m, 20 m, and 36 m in the x, y, and z directions, respectively (Appendix 2, Figure 2). The vent mast height is 6 m. The mesh contained 1.9 million cells. The turbulence is modelled by k-omega turbulence model. The time step is 0.05 s.



FIGURE 2 Computational Domain and Mesh

5 Results

For the original lid design, the simulated maximum speed is 37 m/s, the drag force on the cone is 6.75 N, and the vertical velocity at z = 10 m is 0.516 m/s. For the cone designs, the simulation results are summarized in Appendix 2, Tables 1 to 3.

There are nine (out of 22) cases satisfying the maximum speed constraint as shown in the gray cells in Appendix 2, Table 1. The design P3A2 gave the highest vertical velocity at z = 10 m, resulting in a velocity enhancement of 167% against the original lid design. The design P3A2 passed the check for the drag force and back pressure and is suggested as the optimal design.

Appendix 2, Figure 3 shows the comparison of velocity magnitude between the original lid design and optimal cone design.

Design ID	Al	A2	A3	A4	A5	A6
P1	33.2	32.8	39.5	46.7	-	-
P2	50.2	62	83.4	112.5	148.5	201.4
<i>P3</i>	66.64	82.78	115.4	185.5	286.4	515.1
P4	95.8	143.8	214.1	647.1	-	-
P5	205.2	528.2	-	-	-	-

 TABLE 1

 Simulated Maximum Speed in the Entire Domain (Unit: m/s)

Note: The gray cells denote the cases that satisfied the constraint for the maximum speed and the bold font denotes the optimal design based on the CFD results.

Design ID	A1	A2	A3	A4	A5	A6
<i>P1</i>	0.828	0.724	0.687	0.006	-	-
<i>P2</i>	0.923	0.964	1.002	1.149	1.25	0.93
Р3	1.27	1.38	1.5	1.73	1.51	0.72
P4	1.68	1.82	1.9	0.143	-	-
P5	2.08	2.48	-	-	-	-

TABLE 2 Summary of Simulated Vertical Velocity at *z* = 10 m (Unit: m/s)

Note: The gray cells denote the cases that satisfied the constraint for the maximum speed and the bold font denotes the optimal design based on the CFD results.

TABLE 3					
Summary of Simulated Drag Force on the Cone ((Unit: N	I)			

Design ID	Al	A2	A3	A4	A5	A6
<i>P1</i>	3.28	1.45	0.15	-0.397	-	-
P2	8.87	9.2	15.5	28.5	58.3	113
Р3	14.7	19.9	34.6	102.5	276	1180
<i>P4</i>	28.5	57	140	1780	-	-
P5	165	1168	-	-	-	-

The gray cells denote the cases that satisfied the constraint for the maximum speed Note: and the bold font denotes the optimal design based on the CFD results.

FIGURE 3 Simulated Velocity Magnitude for the Lid Design and Cone Design (P3A2)



Cone design (P3A2)

7 Summary

The gas exit velocity is strongly affected by both the angle and position of the cone design. The optimal cone-shaped vent design (P3A2) selected based on the CFD results achieved an increase of the vertical velocity by 167%.



APPENDIX 3 Examples of Validation Data

1 Introduction

The examples are provided to demonstrate the validation of CFD modeling of gas dispersion. The model parameters presented here are case-specific.

3 Round Jet of Methane

3.1 Case Description

Birch et al. (1984) conducted a series of measurements of compressible jets of natural gas over a pressure range of 1.14 bar to 70 bar. The measurement results demonstrated the theoretical concept of "pseudo-diameter" which can be used to obtain the mean axial concentration in the self-preserving region of a supercritical jet by simply substituting the "true" diameter (d) with the pseudo-diameter (d_{ps}) into the equation for a subsonic round free jet that has been well studied. As illustrated in Appendix 3, Figure 1, a virtual origin displacement (a) is defined as the distance for a high-pressure jet to expand and equilibrate with the ambient condition.

One of the experimental scenarios from Birch et al. (1984) is chosen for the model validation because its condition is the closest to the present application. The gas jet is released upward from an opening with a diameter of 2.7 mm. Appendix 3, Table 1 lists the parameters for the test case. In the CFD simulation, the equilibrated jet condition is applied at the jet inlet since the virtual origin displacement is relatively small (i.e., 3.6D) according to the measurement.



FIGURE 1 Schematic Diagram of a Supercritical Jet Release

Parameter	Symbol	Value
Diameter of opening	D	2.7 mm
Release gas methane content (molar fraction)	Y_i	92% CH4
Release gas molar weight	М	17.32
Release velocity	U_j	408 m/s
Upstream pressure	p_0	1.14 bar
Ambient temperature	Tamb	15°C
Reynolds number	Re	7.0×10^4
Mach number	Ма	0.97

TABLE 1Parameters in the Methane Jet Case

3.3 Model Setup

The computational domain is 37D in the horizontal directions (x and y) and 370D in the vertical direction (z). Appendix 3, Figure 2 shows the three meshes from coarse to fine grids for grid convergence test. The medium mesh has 227,627 cells and the opening is represented by cells with a size of about 0.25D.

The standard *k-epsilon* turbulence model with a modified $C_{\varepsilon 1}$ constant (= 1.6) is applied to improve the modeling of jet decay rate and spreading rate (Pope, 1978). The turbulent Schmidt number is 0.7. The simulation time step is 2×10^{-6} s. The maximum Courant number is about 1.3.





3.5 Results

Appendix 3, Figure 3 displays the simulated and measured centerline velocity and CH_4 molar fraction. The results show that the medium mesh is fine enough to provide grid independent solutions and the CFD model prediction agrees reasonably well with the measurements.

Appendix 3, Figure 4 displays the colormaps of the simulated velocity and CH_4 molar fraction on the central vertical plane (y = 0) from the simulations.

FIGURE 3 Simulated and Measured Velocity and Molar Fraction of CH₄ along the Centerline



FIGURE 4 Colormaps of Simulated Velocity and Molar Fraction of CH₄



5 Variable-density Axisymmetric Jets

5.1 Case Description

The second validation includes cases of variable-density turbulent round jets discharging from a straight circular inner pipe into a weakly confined coflowing air stream in an outer pipe (Appendix 3, Figure 5). These cases were studied experimentally by Djeridane, et al. (1996). The inner pipe has a diameter (D_j) of 26 mm and a length of 600 mm. The diameter of the outer pipe (D_e) is 285 mm. The ratio of pipe diameters is $D_e/D_j > 10$, so the confinement is weak. The purpose of adopting an air coflow is to resolve the problem of seeding at the edges of the jet and provide good conditions for proper velocity measurement using laser-Doppler velocimetry. In addition, this secondary flow is sufficiently weak to avoid radial change during the development of the jet.

The three jets discharging from the inner pipe are helium, air, and CO_2 with specific densities of 0.14, 1.0, and 1.52, respectively. The velocity of the air coflow is 0.9 m/s. The parameters employed in the simulations are listed in Appendix 3, Table 2. The Reynold number (*Re*) in the table is based on the velocity U_j and the inner pipe diameter.



FIGURE 5 Schematic Diagram of the Variable Density Jet Simulations

 TABLE 2

 Parameters of the Varied-density Axisymmetric Jets

Gas	$ ho_{j}/ ho_{e}$	U_j (m/s)	Ue (m/s)	Re
Helium	0.14	32	0.9	7,131
Air	1.0	12	0.9	20,571
CO ₂	1.52	10	0.9	32,261

5.3 Model Setup

The flow in the inner and outer pipes is simulated separately. In the first step, a fully-developed velocity at the end of the inner pipe is obtained. This fully-developed pipe flow is then employed at the jet inlet in the simulation for the outer pipe.

Cylindrical meshes for the inner and outer pipes are generated separately (Appendix 3, Figure 6). For the inner pipe mesh, the grid size is uniform (= 6 mm) in the axial direction. The near-wall cell size on the inner pipe wall is about 1.6 mm. For the outer pipe mesh, the cell size adjacent to the jet exit (z = 0) is refined and gradually stretched in both radial and axial directions to reduce the mesh size. The cell size at the jet exit is about 1.5 mm.

The mesh consists of 594,808 cells in total (i.e., 223,600 cells in the inner pipe and 371,208 cells in the outer pipe).

The standard k-epsilon turbulence model is used. The $C_{\varepsilon l}$ constant is 1.44 for helium and 1.52 for air or CO₂ gas. The simulation time step is 1×10^{-4} s. The maximum Courant number is about 1.5.



FIGURE 6 Computational Domain and Mesh for the Variable Density Jets

5.5 Results

The simulated centerline and radial profiles of velocity and concentration are compared against the measured data as plotted in Appendix 3, Figures 7 through 12. The analytical curves along the jet centerline based on the similarity laws for variable-density jets (Chen & Rodi, 1980) are included in the plots. The analytical formulae are:

$$U_c/U_j = 6.3(\rho_j/\rho_e)^{1/2}(D_j/z)$$

$$C_c/C_j = 5.4(\rho_j/\rho_e)^{1/2}(D_j/z)$$

where

 U_c = centerline velocity

 C_c = centerline concentration

 C_j = jet release concentration

 $\rho_i = \text{density of released gas}$

 ρ_e = density of the ambient co-flow

z = distance from the jet inlet

 U_i and D_i are defined in A3/5.1.





FIGURE 8 Radial Profiles of Simulated Velocity and Mass Concentration of Helium Jet





FIGURE 9 Simulated Centerline Velocity of Air Jet

FIGURE 10 Simulated Centerline Velocity and Mass Concentration of CO₂ Jet



FIGURE 11 Radial Profiles of Simulated Velocity and Mass Concentration of CO₂ Jet





APPENDIX 4 Basic Properties of Methane

Liquefied natural gas (LNG) is composed predominantly of methane (CH₄) and minor quantities of ethane, propane, nitrogen, butane, and other volatile hydrocarbons. LNG vapor is flammable, but the gas-to-air ratio must be between LEL and UEL along with an ignition source for a fire or explosion to occur.

Methane has a lower molecular weight than air. However, the density of methane at its boiling point is much higher than that of air at ambient temperature. When methane is released and mixed with ambient air, the density of the methane gas/air mixture will vary with the methane fraction and temperature of the mixture. Appendix 4, Figure 1 shows the buoyancy of methane gas-air mixture at the ambient temperature of 30°C (86°F). The line of neutral buoyancy is derived from the ideal gas law. The methane gas-air mixture is lighter than the ambient air in the region above the neutral buoyancy line, and heavier in the region below the line. Appendix 4, Figure 2 shows the neutral buoyancy at different ambient temperatures. As seen, the methane gas cloud tends to be more buoyant with lower ambient temperature.

Appendix 4, Table 1 lists an example of basic properties of methane (MKOPSC, 2008; NTP, 1992).



FIGURE 1 Buoyancy of Methane Gas-Air Mixture

FIGURE 2 Neutral Buoyancy of Methane Gas-Air Mixture at Different Ambient Temperatures



TABLE 1 Basic Properties of Methane (CH₄)

Variable	Unit	Value
Molecular weight	kg/kmol	16.04
Freezing point	°C	-182.5
Boiling point at 1 atm	°C	-161.5
Gas density at boiling point	kg/m ³	1.82
Liquid density at boiling point	kg/m ³	425
Specific heat at constant pressure	J/Kg-K	2200
Lower explosive limit (LEL)	% (by volume)	5.0
Upper explosive limit (UEL)	% (by volume)	15.0



APPENDIX 5 Gas Dispersion Exclusion Zone Graph

An exclusion zone graph is created from CFD simulations based on a worst-case scenario defined by the input parameters in Appendix 5, Table 1. Five gas release flow rates at vent exit are considered. Two ambient temperatures (i.e., -25° C and 30° C) are tested. The range of the equivalent release flow rates is based on a tank size study for small gas fueled vessels. The diameter of the vent exit is 0.24 m.

In the simulations, gas release rate is assumed constant, and the depressurization is not taken into account. The exclusion zone presented here is the steady state solution.

This graph may be utilized for pre-screening before conducting a rearrangement or carrying out a more detailed gas dispersion analysis. The CFD simulated exclusion zones are presented in Appendix 5, Figures 1 and 2.

Parameter	Symbol	Value
Released gas	Y_i	100% CH4
Release gas temperature	T_0	-161°C
Release volume flow rate at vent exit	Q	0.9 m ³ /s, 1.8 m ³ /s, 2.7 m ³ /s, 3.6 m ³ /s, 4.5 m ³ /s
Ambient temperature	T_a	–25°C; 30°C
Wind condition	Ua	1 m/s (Pasquill stability class F)

TABLE 1 Gas Release Parameters and Ambient Condition



FIGURE 1 Gas Dispersion Exclusion Zone at Ambient Temperature of –25°C

FIGURE 2 Gas Dispersion Exclusion Zone at Ambient Temperature of 30°C





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