CNG release from pressurized vessel through pressure relief safety device: isentropic flow approach versus CFD model

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ABSTRACT

This paper numerically studies flow characteristics of Compressed Natural Gas (CNG) from a fuel tank of a CNG passenger car through a 3 mm orifice of a temperature triggered pressure relief device (TPRD). The outflow velocity and the methane mass flow are of interest for modelling the gas dispersion both in the vicinity of the orifice as well as further from the leak source. It enables assessing the risk connected with possible accumulation of the explosive gas in enclosures or ignition of leaking gas.

An engineering approach of isentropic nozzle flow was compared to the results of a 2D CFD simulation over the whole range of the reservoir working pressure 200 bar (full fuel tank). The pressure in the reservoir was assumed constant. CNG was approximated as pure methane. Methane in the reservoir was set at ambient temperature as well as the surrounding air.

Both models predict the same trends both in the methane outflow velocity and mass flow through the orifice. Excellent correspondence between both models was found up to reservoir pressure 50 bar. Above this value, isentropic model predicts about 10 % higher outflow velocity, and even smaller difference was found in the predicted methane mass flow. Mass flow prediction of the isentropic model is, however, strongly dependent on the discharge coefficient.

For reservoir pressures between 50 to 200 bar, the Mach number predicted by CFD was in the range from 3.5 to 6 which corresponds to a transition region between super and hypersonic flow. Even at such high speed flow, CFD predictions were consistent with the isentropic nozzle flow theory and in general, the correspondence between both models is very satisfactory.

KEYWORDS: CNG; gas dispersion; modelling; CFD; isentropic flow
INTRODUCTION

During the last two decades, the amount of CNG vehicles steadily increase. CNG vehicles are nowadays commonly present in the everyday traffic. Presence of the pressure vessel on board the vehicle and the risk of CNG leak either from the high or low pressure pipeline, however, present a safety concern. To prevent the critical pressure buildup, each fuel tank has to be equipped with the temperature triggered pressure relief device (TPRD) with activation temperature of 110±10 °C. In case of the TPRD activation or leak from the high pressure pipeline, large amount of CNG is released through a small orifice or hole in a relatively short time to the ambient atmosphere. The outflow velocity and the CNG mass flow from the fuel system to the surroundings are of key importance for further analysis of gas dispersion, ignition probability analysis, design of the detection and ventilation systems etc.

Outflow of gas from pressurized vessel to ambient atmosphere

Working pressure in the passenger CNG vehicles is usually 200 bar. With such a high pressure difference, the resulting flow from a pressurized environment to the ambient well exceeds the speed of sound. Compressibility effects play significant role and must be considered in order to predict the flow. Isentropic models [1] are often used to describe the flow characteristics of both subsonic and supersonic compressible flows through a nozzle/orifice. Isentropic flow is any flow that is adiabatic and reversible. No friction or dissipative effects are considered. The outflow characteristics can be calculated based only on the stagnation state characteristics (reservoir pressure). The main assumption of isentropic flow is that it is a reversible process. When the gas that flows through the nozzle/orifice/hole is turned abruptly at the exit plane, shock waves emerge, and highly underexpanded jet is created [2]. The flow is irreversible, and isentropic relations are no longer valid. Another option to describe the flow characteristics of compressible fluid is to use CFD. The advantage of the CFD model is that compared to isentropic flow models it also provides the spatial information about the flow and structure of the underexpanded jet [3]. Friction and dissipative losses are accounted. The flow regimes can be distinguished based on the Mach number. Common CFD solvers are validated for supersonic flow applications typically characterised by the Mach number in the range 1.2 to 5. The outflow velocities from the full fuel tank are expected to locally exceed Mach 5 switching to hypersonic flow regime. At such flow speed, turbulence modelling becomes a significant concern, and the approximation of the gas thermodynamics behaviour as ideal becomes questionable. However, outflow velocity measurements at super or hypersonic speed is extremely difficult to perform. Validation of the CFD model compared to experimental data is thus rarely possible. This work compares outflow velocity and gas mass flow of methane from pressurized reservoir through 3 mm orifice as predicted by the isentropic flow model and 2D CFD model. These characteristics are of significant importance serving as a boundary condition to CNG leak risk analysis. The fuel leak results in highly momentum driven flow. Jet fires may be observed and present significant safety concern. At the same time due to strong mixing the gas leaving the bottom region of the car looses big part of its momentum. From the long term view the proper estimate of the fuel mass flow is crucial for modelling gas dispersion further from the leak source.

ISENTROPIC FLOW MODEL

The outflow velocity $v$ from the pressure vessel can be derived from the principle of energy conservation [4]. Assuming pressure and density of the isentropic flow are related as $p \rho^\gamma$ = constant, Bernoulli equation for ideal compressible fluid, where subscript zero denotes the conditions in the pressure reservoir (stagnation state), is obtained

$$\frac{v_0^2}{2} + \frac{y \cdot p_0}{\gamma - 1 \cdot \rho_0} + h_0 g = \frac{v^2}{2} + \frac{y \cdot p}{\gamma - 1 \cdot \rho} + h g.$$  

(1)

Assuming the contribution of the $hg$ term in Eq. 1 is negligible and the fluid velocity in the vessel is negligible compared to the outflow velocity ($v_0 \approx 0$), the outflow velocity can be calculated as

$$v = \sqrt{\frac{2y \cdot p_0}{\gamma - 1 \cdot \rho_0} \left[ 1 - \frac{p}{p_0} \right]^{\frac{y - 1}{y}}}. $$  

(2)

Equation 2 is known as Saint-Venant-Wantzel equation. $\gamma$ is an isentropic exponent (isentropic expansion coefficient) which is a ratio of ideal gas isobaric and isochoric specific heat. In this work, $\gamma$ for methane was set 1.304 (calculated at ambient conditions) independent of temperature.
Theoretical mass flow from the reservoir can be derived as \( \dot{m} = \rho v A \). \( A \) is the outflow area. Substituting for \( \rho \) from the isentropic relation \( p/p_0 = (\rho/\rho_0)^{\gamma} \), and multiplying by discharge coefficient \( C_d \) yields equation for the real mass flow in the subsonic region
\[
\dot{m} = C_d A p_0 \frac{2y M}{\gamma - 1} \left( \frac{p}{p_0} \right)^{\frac{\gamma + 1}{\gamma - 1}}. \tag{3}
\]

After reaching the critical condition, the flow is choked. For calculating the mass loss in the supersonic region, velocity corresponding to the critical pressure ratio is substituted to the continuity equation resulting in relation for mass flow through orifice in the supersonic region as
\[
\dot{m} = C_d A p_0 \frac{y M}{\gamma + 1} \left( \frac{p}{p_0} \right)^{\frac{\gamma + 1}{\gamma + 1}}. \tag{4}
\]

For the comparison with the mass flow predicted by the CFD model through the orifice depicted in Fig. 1., discharge coefficient 0.98 was used (recommended value for the rounded type orifices [5]).

2D CFD MODEL

A commercially available CFD solver ANSYS CFX 17.2 was used to perform all CFD simulations. Computational domain is shown in Fig. 1. Methane is supplied from the reservoir to the surroundings through the 3 mm orifice (real orifice size of one of the commercially used passenger vehicle TPRD). The created underexpanded jet is free and supposed to be axisymmetric. 2D simulation was thus used to save computational cost. Other possibility to save computational time is to create the case in cylindrical coordinates, which is close to the real reservoir and orifice geometry, and use axial symmetry and thus divide the mesh size by two. However, ANSYS CFX does not have a 2D-axisymmetric solver (as introduced in ANSYS FLUENT). Concerns about the capability of the axisymmetric solver to capture the behaviour of the supersonic to hypersonic flow on the axis of symmetry were also made. 2D Cartesian coordinates case was created although the curvature of the orifice is neglected.

The domain representing the ambient environment is 4×4 meters initially filled with air having 20 °C at ambient pressure 1.01325 bar. Pressure reservoir is not considered in the domain, only a section of the outflow path close to the orifice of the TPRD where the inlet boundary condition is defined (see the detail in Fig. 1.). An unstructured hexahedral mesh with boundary layer on the walls was created for whole domain in ANSYS ICEM CFD 17.2. The first element height was equal 1·10⁻⁵ m which proved to be sufficient for the SST k-\( \omega \) turbulent model according to the \( y^+ \) values on walls.

Fig. 1. Simplified computational domain representing the outflow from a pressure reservoir through 3 mm orifice to the surroundings.
Inlet boundary condition (which corresponds to reservoir conditions) is defined as a total pressure of pure methane in the reservoir having 20 °C (T₀). Pressure (p₀) is assumed to be constant. 10 cases were simulated: 1.5, 5, 10, 30, 50, 75, 100, 150 and 200 bar. Outlet boundary condition is of type opening with constant static pressure and ambient temperature 20 °C. Thermodynamic properties of both air and methane were governed by ideal gas law.

All performed simulations were steady state. The transient effects of mixing and turbulent structures cannot be predicted. However, for the purpose of this study, the global trend of the outflow velocity along the jet structure can be well captured by the steady state simulation and again significantly save computational cost.

The two-equation eddy-viscosity SST k-ω turbulent model with an automatic wall function was used for turbulence modelling. Second order accurate approximations for all terms in the governing equations were applied. Due to the convergence issues various expert parameters for linear solver and advanced options for solver control were tested.

RESULTS

For the comparison of the outflow velocities (Fig. 3), maximum velocity found along the jet structure predicted by CFD was used. Isentropic model predicts the characteristics of the flow, as a result of the pressure difference of reservoir and ambient conditions, with no spatial resolution. From this point of view, isentropic model is a 0D model.

Critical pressure for pure methane leaking to ambient atmosphere of 1.01325 bar with isentropic coefficient 1.304 is approximately 1.86 bar. Above this value, the flow is supersonic. The correspondence between two models is excellent up to 10 bar. The outflow velocity is rapidly increasing up to reservoir pressure 10 bar. After 50 bar, the increase in the outflow velocity is small, as predicted by both models. Isentropic model predicts about 10 % higher outflow velocities, but the overall trend is the same for both models.

Mach number is a strong function of temperature. Due to the gas expansion, the temperature of the gas drops significantly. It is thus difficult to compare the flow velocities as a function of reservoir pressure in terms of Mach number. However, for the 50 bar simulation, the maximum velocity predicted by CFD along the centreline of the jet corresponds to approximately 3.6 Mach at temperature -173 °C. Both models predicts the flow between 50 bar and maximum pressure of 200 bar between 3.5 to 6 Mach which corresponds to the transition between super and hypersonic region.

In terms of the mass flow, similar trends to velocity are observed (Fig. 4). The correspondence between models is excellent up to 50 bar. For higher reservoir pressure, there is a slight disagreement. The value of discharge coefficient 0.98 used in the isentropic model well represent the nozzle geometry used in the CFD model. As expected from Eq. 4., the mass flow above the critical conditions is a linear function of reservoir pressure.
Maximum mass flow of methane at 200 bar through the orifice is approximately 10 g/s. It is necessary to point out that the outflow area is not the whole area of the orifice but area of the rectangle being 3 mm high and 1 computational cell thick as the simulation is only 2D. When scaled to the round orifice 3 mm in diameter, the mass flow is approximately 240 g/s. The same value was obtained from the isentropic model with discharge coefficient 0.98.

Experimental work measuring the mass flow through TPRD at 200 bar was performed as a part of the previous research. Experiments were transient. The pressure decrease is extremely fast (the pressure drops in five seconds about 50 bar). The estimate of the steady state mass loss rate to compare with the simulation is based on fitting the transient data and divided by 6 (number of TPRD orifices). The measured value of the mass loss rate through one 3 mm orifice at 200 bar pressure was experimentally estimated to be around 150 g/s. Considering, there will be significant pressure drop in the outflow path through the solenoid valve to TPRD and accounting for other nonideal factors that would be included in the discharge coefficient, mass flow predicted by both models corresponds in the order of magnitude with the experiments and literature values [6, 7].
CONCLUSIONS

The outflow velocity and methane mass flow predicted using isentropic model and 2D CFD model show very good correspondence over the whole range of fuel tank working pressure. Even at the hypersonic flow regime the CFD predictions seems consistent with the results obtained using isentropic flow theory of compressible fluid nozzle flow. However, it needs to be stressed out that validation of the outflow velocity over experimental data was not performed. Obtained mass flows were found to correlate with literature and our previous experiments.

Isentropic models provided easy to use and fast engineering estimates of the outflow characteristics of the gas leak from the pressurized vessel that can serve as a boundary condition for further analysis. The proper value of discharge coefficient is, however, crucial for the real mass flow estimates and may not be easily established for fuel leaks through TPRD or leak from the high pressure fuel line. However, it is generally recognized that using the idea of ideal mass flow is on the “safe side” predicting higher mass flow.

CFD modelling of compressible and supersonic flow is time consuming and requires experienced user. Convergence issues were repeatedly encountered as the nature of the problem is highly transient, but the simulation was performed as steady state. On the other hand CFD provides complex insight on the flow characteristics along the nozzle and further along the exit plane of the emerged underexpanded yet.

NOMENCLATURE LISTING

| Symbol | Description       |
|--------|-------------------|
| $A$    | area (m$^2$)      |
| $C_d$  | discharge coefficient |
| $g$    | gravitational constant (m$^2$/kg/s$^2$) |
| $h$    | elevation (m)     |
| $M$    | molar mass (kg/mol) |
| $p$    | pressure (Pa)     |
| $R$    | universal gas constant (J/mol/K) |
| $T$    | temperature (K)   |
| $v$    | velocity (m/s)    |
| $\gamma$ | isentropic exponent |
| $\rho$ | density (kg/m$^3$) |
| $h_{res}$ | reservoir – stagnation state |

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