

Analysis of Reservoir Pressure Decay, Velocity and Concentrations Fields of Natural Gas Venting from Pressurized Reservoir into the Atmosphere

2011-01-0252

Published
04/12/2011

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doi:[10.4271/2011-01-0252](https://doi.org/10.4271/2011-01-0252)

ABSTRACT

Compressed natural gas (CNG) currently is used as an alternative fuel for internal combustion engines in motor vehicles. This paper presents results of an analysis of leaks from a model isolated section of CNG fuel system. Discharge of CNG was modeled as vent flow of a real gas hydrocarbon mixture through an orifice from a reservoir with finite volume. Pressures typically used in CNG fuel systems result in choked flow for gas venting directly to atmosphere, producing an under-expanded, momentum-dominated, turbulent free jet with well defined velocity and concentration fields. This paper presents results of analyses of reservoir pressure decay, and vent flow and concentrations fields for CNG venting from a pressurized reservoir into the atmosphere. A combination of empirically-derived analytical relationships and detailed two-dimensional high resolution computational fluid dynamic modeling was used to determine the velocity and concentrations fields of the resulting CNG jet. The internal volume and initial gas pressure used in this analysis are in the range of an isolated rail in a CNG fuel system. These concentration and velocity fields are then used to assess ignition probability and flame stability.

INTRODUCTION

Compressed Natural Gas (CNG) fuel systems in motor vehicles consist of a high pressure tank or tanks, a fuel rail on the engine, and some type of plumbing that connects these components. CNG fuel systems also contain one or more pressure regulators used to step-down pressure from the tank to the fuel rail, and one or more shut-off valves used to

isolate high pressure sections of the fuel system from lower pressure sections of the fuel system. This paper presents an analysis of the probability of ignition of gas leaking from a low pressure section of a CNG fuel system, for example the fuel rail, isolated from the fuel tank by a closed shut-off valve. First, the pressure decay in and mass flow rate from the reservoir were determined using two models of isentropic flow through an orifice. Pressures typically used in CNG fuel rail result in super-critical flow when venting to atmosphere, which creates a turbulent, momentum-dominated under-expanded jet. Two-dimensional concentration and velocity fields of the resulting vent flow as a function of reservoir pressure were determined using non-dimensional relationships developed from the study of turbulent free jets of natural gas. These results are compared to concentration and velocity fields determined using a two-dimensional (2-D) high resolution computational fluid dynamic (CFD) model of gas flow venting from a pressurized pipe. The high resolution CFD model provided detailed information about the shock structure, and the resulting pressure, temperature, and density fluctuations in the jet expansion region which could not be obtained from existing non-dimensional empirical relationships. The CFD model also was used to determine concentration and velocity fields of the jet.

The internal volumes and working pressures used in this analysis do not represent a CNG fuel system in a specific vehicle. Internal volumes and working pressures in a specific vehicle will depend on the design of the fuel system and intended application of the vehicle, and most likely will be

different from the internal volumes and working pressures used in the analysis presented in this paper.

COMPOSITION OF NATURAL GAS

Physical properties of natural gas such as compressibility, density or molar volume, enthalpy, and entropy, as well as its phase behavior depend on its composition. Natural gas is predominantly methane, but may contain C2 through C6+ hydrocarbons, carbon dioxide, nitrogen, oxygen, hydrogen, and other trace gases. The composition, and thus the physical properties of natural gas can vary with source, season, and processing. As an example, [Table 1](#) shows a the variation in natural gas composition of natural gas supplied by Union Gas, a major Canadian natural gas storage, transmission and distribution company with sources from Western Canada, Ontario, and the United States [1]. This range of composition also is typical of natural gas supplied by ANR Pipeline Company, which supplies natural gas to utility companies throughout the US and Canada [2]. Natural gas from other sources can have an appreciably different composition than shown in [Table 1](#).

Table 1. Natural Gas Composition

Component	Natural Gas	
	Range	NG-1
	(mole %)	(mole %)
Methane (C ₁)	87 – 96	95.496
Ethane (C ₂)	1.5 – 5.1	2.232
Propane (C ₃)	0.1 – 1.5	0.368
n-Butane (C ₄)	0.01 – 0.3	0.070
iso-Butane (C ₄)	0.01 – 0.3	0.054
n-Pentane (C ₅)	trace – 0.04	0.019
iso-pentanes (C ₅)	trace – 0.14	0.025
Hexanes + (C ₆ +)	trace – 0.06	0.046
Nitrogen (N ₂)	0.7 – 5.6	0.615
Carbon Dioxide (CO ₂)	0.1 – 1.0	1.075
Oxygen (O ₂)	0.01 – 0.1	0.000
Hydrogen (H ₂)	trace – 0.02	0.000

A study, published in 1994, indicated the mean methane concentration in natural gas samples taken throughout the continental US was 93.0%, with a minimum of 55.8% and a maximum of 98.1% [3]. Another study, published in 2006, indicated the average methane concentration of CNG available at vehicle fueling stations in California was 93.4% [4]. Natural gas with relatively low methane and high content of C2 through C6+ hydrocarbons may be less desirable for

use as a fuel in CNG vehicles as pressure cycling can result in condensation of the heavier hydrocarbons. The column labeled NG-1 in [Table 1](#) shows the composition of natural gas, determined by gas chromatographic analysis, of fuel available at a DTE Energy CNG fueling facility in Willow Run, Michigan on January 28, 2010 [5]. Physical properties based on this chemical composition (labeled NG-1) were used to determine vent flow in the analyses presented in this paper.

EQUATION OF STATE

In principle, thermodynamic properties of a natural gas can be measured directly. As direct measurement is time consuming at best, and impractical in most cases, thermodynamic properties of a natural gas are calculated from the gas composition using an equation of state (EOS).

The simplest equation of state is the Ideal Gas Law. Implicit in the Ideal Gas Law are assumptions that molecules in the gas phase occupy zero volume, collisions between molecules in the gas phase and the wall of a container are perfectly elastic, and there are no intermolecular interactions (attractions or repulsions) between molecules in the gas phase. Although these assumptions are clearly wrong for all real gases, the Ideal Gas Law yields reasonably accurate values of density or molar volume, for example, for most gases near normal atmospheric pressure and temperature. However, errors in density, defined as the difference between calculated value of density and the real (measured) value of density of a substance, using the Ideal Gas Law can be substantial for gases at extreme pressures and temperatures, and for super critical fluids. Moreover, the Ideal Gas Law does not account for thermodynamic properties of real gases.

More accurate values for fluid properties are obtained by using equations of state that account for real gas behavior. A number of methods based on various cubic equations of state have been used in the oil and gas industry to derive more accurate thermodynamic properties of natural gas mixtures based on gas composition data [6, 7]. Methods based on Helmholtz free energy EOS yield the most accurate thermodynamic properties of gas mixtures from composition over a wide range of temperatures and pressures [8,9,10]. A method described in American Gas Association Report 8 [8] currently is the standard in the natural gas industry for calculating the volumetric and caloric properties of hydrocarbon mixtures, but is valid for the gas phase only and does not address phase equilibrium. Recently, research sponsored by The Groupe European de Recherches Gazieres (The European Gas Research Group), abbreviated as GERG, has lead to the development of methodology based on Helmholtz free energy EOS that yields highly accurate thermophysical properties of pure compounds and mixtures over the gas, liquid, and supercritical fluid regions [9]. REFPROP V 8.0, a program available from The National

Institutes of Standards and Technology (NIST), uses an approach based on Helmholtz free energy EOS similar to GERG2004 [10], and was used to determine thermodynamic properties of natural gas (NG-1 in Table 1) for the analysis presented in this paper.

LEAKAGE FROM AN ISOLATED CNG FUEL SYSTEM SECTION

An isolated section of a CNG fuel system was modeled as a pressurized reservoir with an internal volume of 0.0003 m³ (300 cm³) containing NG-1 (Table 1) at a settled temperature and pressure of 288°K (15°C) and 1.0 MPa (10 bar), respectively. Fuel venting from a leak in this reservoir was modeled as isentropic flow of a compressible fluid through an orifice into initially stagnant air at a temperature of 288°K (15°C) and pressure of 0.101325 MPa.

GAS FLOW FROM AN ORIFICE

At low internal pressures, the mass flow and exit velocity of gas is a function of the difference in internal and external pressures, in this case the difference between the initial vessel pressure and atmospheric pressure. Flow is initially choked and the fluid velocity in the orifice (exit velocity) is sonic and independent of internal pressure when [11,12,13]:

$$\frac{P_1}{P_{atm}} \geq \left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}} \quad (1)$$

The isentropic expansion factor typically is approximated as the ratio of the isobaric heat capacity to isochoric heat capacity, and assumed to be invariant with temperature and pressure largely because of lack of data on the dependence of heat capacities with temperature and pressure for most gases. For real gases, the isentropic expansion factor is usually slightly less than C_p/C_v , and varies with temperature and pressure. Published values of C_p/C_v for natural gas range from approximately 1.3 to 1.4. The isentropic expansion factor for NG-1 at $T = 288^\circ\text{K}$ and $P = 1.0$ MPa determined using REFPROP V 8.0 was 1.3116, which results in a critical pressure of 0.186 MPa. As the initial pressure in the fuel system is greater than 0.186 MPa, flow through the orifice is initially super-critical, is limited to the sonic velocity of NG-1 at the conditions of temperature and pressure in the orifice, and remains choked until the pressure in the fuel system falls below 0.186 MPa. The instantaneous mass flow rate, temperature, pressure, and density of gas in the orifice are given by equations 2, 3, 4, 5, 6, respectively [11].

$$Q = AC_D \sqrt{\gamma P_1 \rho_1 \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-2}}} \quad (2)$$

$$P_2 = P_1 \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma+1}} \quad (3)$$

$$T_2 = T_1 \left(\frac{2}{\gamma+1}\right) \quad (4)$$

$$\rho_2 = \rho_1 \left(\frac{2}{\gamma+1}\right)^{\frac{1}{\gamma+1}} \quad (5)$$

$$V_2 = \sqrt{\frac{\gamma R T_2}{M_w}} \quad (6)$$

Table 2 shows values of instantaneous initial mass flow rate, pressure, temperature, density, and velocity for NG-1 reservoir at an initial pressure $P_1 = 1.0$ MPa through 0.1, 0.2, 0.5, 1.0, 2.0 mm diameter orifices determined using equations (2), (3), (4), (5), (6).

Table 2. Initial Mass Flow Rate, Pressure, Temperature, Density, Velocity, Densimetric Froud Number, and Reynolds Number for Isentropic Flow of NG-1

	Orifice Diameter (mm)				
	0.1	0.2	0.5	1.0	2.0
Q (g/s)	0.012	0.048	0.300	1.20	4.80
P ₂ (MPa)	0.545	0.545	0.545	0.545	0.545
T ₂ (K)	250	250	250	250	250
ρ ₂ (kg/m ³)	4.524	4.524	4.524	4.524	4.524
V ₂ (m/s)	398	398	398	398	398
Fr ^a	20,600	14,600	9,200	6,500	4,600
Re ^b	6,600	13,200	33,000	66,000	132,000

$$^a Fr = u / (gd((\rho_{atm} - \rho_{NG-1})/\rho_{NG-1}))$$

$$^b Re = (u\rho d)/\mu$$

GAS DISCHARGE FROM A RESERVOIR

The discharge rate from a pressurized reservoir decreases as the pressure in the reservoir decreases. A number of publications present quantitative relationships for the time-dependence of the pressure and temperature in the reservoir and in the orifice, and the mass flow rate for gas discharging from a pressurized reservoir [14, 15, 16, 17]. These relationships were derived assuming a reversible, adiabatic (isentropic) expansion of a non-condensable ideal gas. The assumption that gas flow through an orifice is isentropic is reasonable for rapid depressurization of a pressurized reservoir. However, heat transfer from the reservoir to the gas during a slow depressurization may result in deviation from a purely isentropic process. Moreover, a complex mixture such as natural gas may undergo phase changes during depressurization as the pressure and temperature of the gas in the reservoir and orifice decrease during discharge.

A method for calculation of the time-dependent flow rate during rapid depressurization of a pressurized reservoir for an isentropic process based on recently available EOS allows not only a rigorous evaluation of flow conditions of a real gases, but evaluation of the phase behavior of a real gas during the venting process [18]. Characterization of the discharge process by this method involves solution of the following equations for a real gas:

$$\frac{H_0(P_0, T_0, \bar{C})}{M_W} = \frac{H(P, T, \bar{C})}{M_W} + \frac{v^2}{2} \quad (7)$$

$$S_0(P_0, T_0, \bar{C}) = S(P, T, \bar{C}) \quad (8)$$

$$u \leq c(P, T, \bar{C}) \quad (9)$$

Figures 1, 2, 3 show plots of the time dependent pressure, temperature and mass flow rates for discharge of NG-1 (Table 1) from a reservoir ($V = 0.0003 \text{ m}^3$, $P_i = 1.0 \text{ MPa}$, and $T_i = 288^\circ\text{K}$) through an orifice ($d = 0.5 \text{ mm}$) determined using two models for gas discharge from a pressurized reservoir.

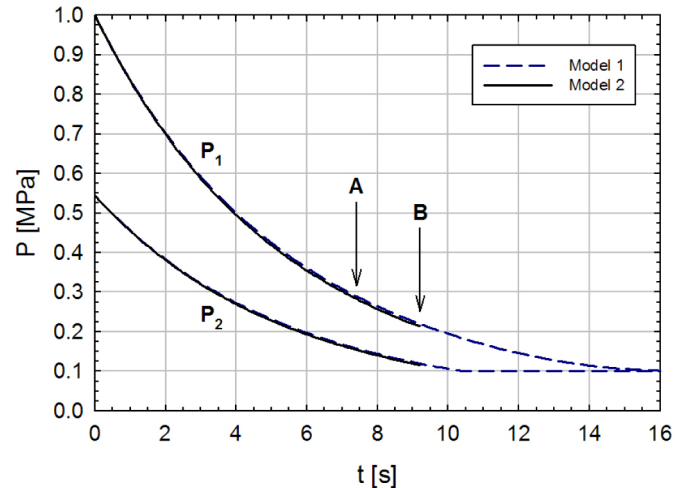


Figure 1. Plots of gas pressure in the reservoir (P_1) and in the orifice (P_2) vs. time for discharge of NG-1 ($V = 0.0003 \text{ m}^3$, $P_1(0) = 1.0 \text{ MPa}$, and $T_1(0) = 288^\circ\text{K}$, and $d = 0.5 \text{ mm}$). Condensation in the orifice (A). Condensation in the reservoir (B).

Model 1 was the method of calculating gas discharge rated for super-critical and sub-critical described in reference 16, where the isentropic expansion factor for NG-1 was held constant a value of $\gamma = 1.3038$ (determined using REFPROP for NG-1 at $T = 288^\circ\text{K}$ and $P = 1.0 \text{ MPa}$). Model 2 was the method described in reference 18, using REFPROP to determine time-dependent thermodynamic properties of NG-1 in the reservoir and in the orifice during discharge. In both models $C_D = 0.85$.

Figures 1 and 2 show that Model 1 yielded slightly greater values P_1 , P_2 , T_1 , and T_2 than Model 2, and that differences in these parameters increased over time (increasing mass loss from the reservoir). Results not presented here show that differences between the predictions of Models 1 and 2 increase if either the initial pressure of gas in the reservoir is increased from 1.0 MPa or the initial temperature of gas in the reservoir is increased from 288°K. Thus, differences in reservoir and orifice pressures and temperatures shown in Figures 1 and 2, respectively, are the result of the non-ideal behavior of natural gas with a composition NG-1.

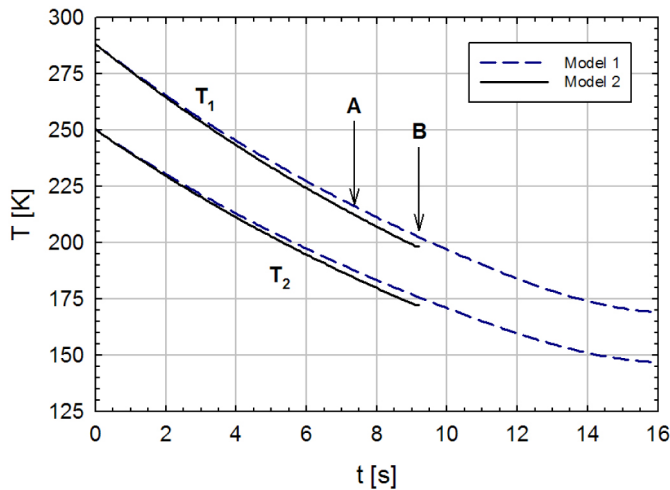


Figure 2. Plots of gas temperature in the reservoir (T_1) and in the orifice (T_2) vs. time for discharge of NG-1 ($V = 0.0003 \text{ m}^3$, $P_1(0) = 1.0 \text{ MPa}$, $T_1(0) = 288^\circ\text{K}$, and $d = 0.5 \text{ mm}$). Condensation in the orifice (A). Condensation in the reservoir (B).

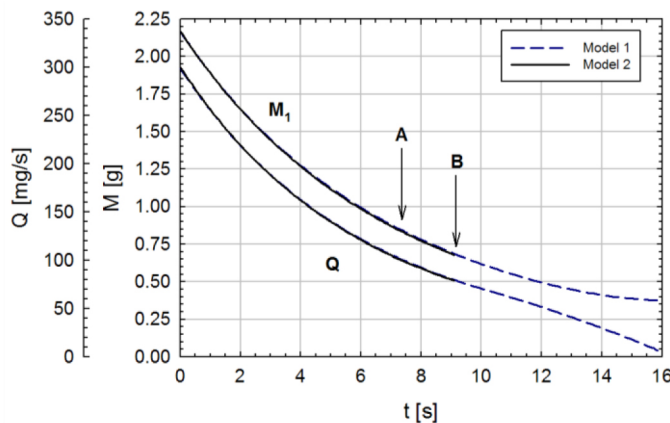


Figure 3. Plots of mass flow rate from the reservoir (Q) and mass remaining in the reservoir (M_1) vs. time for discharge of NG-1 ($V = 0.0003 \text{ m}^3$, $P_1(0) = 1.0 \text{ MPa}$, $T_1(0) = 288^\circ\text{K}$, and $d = 0.5 \text{ mm}$). Condensation in the orifice (A). Condensation in the reservoir (B).

Model 1 indicated complete discharge of the reservoir containing NG-1 initially at $P_1(0) = 1.0 \text{ MPa}$ and $T_1(0) = 288^\circ\text{K}$ took 16.3 s, with transition from super-critical to sub-critical flow occurring at 10.4 s when $P_1 = 0.186 \text{ MPa}$ and $P_2 = P_{\text{atm}} = 0.101325 \text{ MPa}$ (Fig. 1). Plots of T_1 and T_2 showed decreasing gas temperatures in the reservoir and in the orifice, respectively, with no noticeable inflection at the transition from super-critical to sub-critical flow (Fig. 2). The initial mass flow rate of gas from the reservoir was 300 mg/s and, as expected, decreased to 0 mg/s when $P_2 = P_{\text{atm}}$. About 17% of the initial mass of CNG remained in the reservoir

when reservoir pressure equilibrated with atmospheric pressure and discharge ceased (Fig. 3).

Time-dependent gas pressures in the reservoir and in the orifice, and the mass flow rate of gas from the reservoir during discharge determined using Model 2 were nearly identical to those determined using Model 1 (Fig.'s 1 and 3). Time-dependent gas temperatures in the reservoir and in the orifice determined using Model 2 initially were nearly identical to those determined using Model 1, but decreased at a slightly greater rate during discharge (Fig. 2). The agreement between results of these models is somewhat surprising as Model 1 was based on isentropic flow of a non-condensable gas where constant values of $\gamma = 1.3038$ and $c = 424.82 \text{ m/s}$ (determined for NG-1 using REFPROP at the initial pressure and temperature of the gas in the reservoir) for the entire discharge.

Whereas values of γ and c used in Model 2 were determined using REFPROP for instantaneous conditions in the reservoir and orifice ($1.3038 \leq \gamma \leq 1.3217$ for NG-1 in the reservoir, $1.3140 \leq \gamma \leq 1.3257$ for NG-1 in the orifice, and $397.9 \leq c \leq 333.6 \text{ m/s}$ for NG-1 in the orifice during super-critical flow).

Another difference between the model predictions shown in Figures 1, 2, 3 is the ability of Model 2 to predict condensation during the discharge. The derivation of equations for determination of time-dependent properties of the gas during discharge used in Model 1 assumed the gas was non-condensable [16]. In contrast, the approach used in Model 2 can be used to determine the phase behavior of the gas during discharge. Figure 4 is a phase diagram for NG-1 determined using REFPROP [10].

NG-1 is a superheated vapor in the reservoir before the start of discharge, ($T_c = 198.042^\circ\text{K}$, $P_c = 5.04192 \text{ MPa}$, and $\rho_c = 162.69 \text{ kg/m}^3$). Components in NG-1 will start to condense when the pressure and temperature of the gas is within the two-phase region defined by the vapor and liquid saturation lines (Fig. 4). For isentropic expansion of NG-1 starting at $T_i = 288^\circ\text{K}$ and $P_i = 1.0 \text{ MPa}$ (solid blue line in Fig. 4), this occurs in the orifice at 7.4 s after the start of discharge (A in Fig.'s 1, 2, 3) when $T_2 = 184^\circ\text{K}$ and $P_2 = 0.154 \text{ MPa}$, and in the reservoir at 9.2 s after the start of discharge (B in Fig.'s 1, 2, 3) when $T_1 = 198^\circ\text{K}$ and $P_1 = 0.214 \text{ MPa}$.

The initial temperature and pressure of the gas in the reservoir will affect the phase behavior of the gas during discharge. The temperature-pressure trajectory of NG-1 during isentropic expansion from $T_i = 325^\circ\text{K}$ and $P_i = 1.0 \text{ MPa}$ is shown in Figure 4 to illustrate this point. For gas discharging from the reservoir under these conditions, components in the venting gas would start to condense in the orifice 11.9 seconds after the start of discharge when $T_2 = 173^\circ\text{K}$ and $P_2 = 0.070 \text{ MPa}$, and residual gas in the reservoir