USE OF SUITABLE EQUATION OF STATE FOR THE CONVERSION OF VOLUMETRIC TO MASS FLOWRATE IN NGV REFUELING MEASUREMENT

(Date received: 19.6.2006)

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ABSTRACT

Natural Gas Vehicle (NGV) is not new in the industry; however, it is becoming an uprising issue owing to the multitude advantages natural gas posses compared to the conventional fuel. The challenges, on the other hand, are putting in place an NGV refueling facility and keeping the cost of natural gas operated vehicles competitive with conventional vehicles. One of the identified cause for the dearly NGV refueling station installation cost is the mass measurement device, Coriolis flow meter, used in each station. This research is aimed at finding and implementing a cost effective alternative to the Coriolis flow meter. A typical volumetric flow meter i.e., turbine, orifice and vortex is much lower in price but does not produce measurement in the natural gas trading unit. To compensate for this, a conversion tool based on an Equation of State (EOS) is developed. In this method, mass flowrate of natural gas is calculated using the volumetric flowrate measured by volumetric flow meter, whilst temperature and pressure of the flowing gas are fed into the conversion tool. Based on results, it is found that the developed conversion tool is able to compute the mass flowrate of natural gas with reasonably average error which is 2.66% compared to the actual measurement using Coriolis flowmeter.

Keywords: *Coriolis Flow Meter, Equation Of State, NGV Refueling Station*

1.0 INTRODUCTION

Automotive industry is one of the fastest growing industries in the world. In 2005, Daud [1] reported that in Malaysia for the past ten years, the average vehicle population growth is about 7% per annum. The fast growing industry enables people to travel faster than before and a vehicle has become an essential tool for mankind. However, the increasing number of vehicles also resulted in severe environmental problems. Emissions from millions of cars and light-duty trucks, almost exclusively operating on gasoline and diesel fuel, are major contributors to this problem. In addition, heavy-duty trucks and buses using diesel fuel are major sources of particulates (small unburned particles of hydrocarbons and sulfur) and *nitrogen oxide* (NO_x) emissions in urban areas. Particulates are a special concern because the public is frequently exposed to them and a research conducted by Bechtold in 1997 [2] suggested that particulates have cancer-causing potential and it could cause significant respiratory problems.

Alternative vehicle fuels such as natural gas have long been proposed as a way to provide significant air quality benefits over liquid petroleum fuels. Significant advances have been made in the past few years that have highlighted the efficiency and emissions potential of *NGV* [3-7]. In transportation sector, natural gas is becoming more important. *NGV* has many overwhelming advantages in comparison with traditional means of transportation using gasoline and diesel. It is more environmentally friendly [3-5], safer and lower fuel cost compared to gasoline powered vehicle. Nylund and Erkkila [6] reported that *NGV* was found to give NO_x emission of about 75% less, compared to gasoline powered vehicle. This is further supported by an emission study conducted at Argonne National Laboratory [7] that showed natural gas with CO_2 emissions of 140gm CO_2 eq/km, gasoline at 176gm CO_2 eq/km, and diesel at 147gm CO_2 eq/km.

To date, there are only 40 *NGV* refueling stations to cater for 15,600 *NGVs* in Malaysia [1]. To encourage public transport operators to use natural gas, more *NGV* stations would have to be built. Lack of refueling facility is the major obstacles to the growth of *NGV* usage. The problem is not only faced by Malaysia but also other countries in the world. High cost of its metering system is believed to be one of the main constraints to the growth of *NGV* refueling facility. The high cost of the metering system is mainly due to very expensive flow meter used in the metering system that is the Coriolis flow meter. Current technology used in *NGV* refueling equipment's metering system is by using Coriolis mass flow meter [8]. This meter uses the Coriolis Effect to measure the amount of mass moving through the element. The substance to be measured runs through a U-shaped tube as shown by Figure 1 which vibrates in a perpendicular direction to the flow. Fluid forces running through the tube interact with the vibration, causing it to twist. The greater the angle of the twist, the greater is the flow based on momentum change that is related to mass.

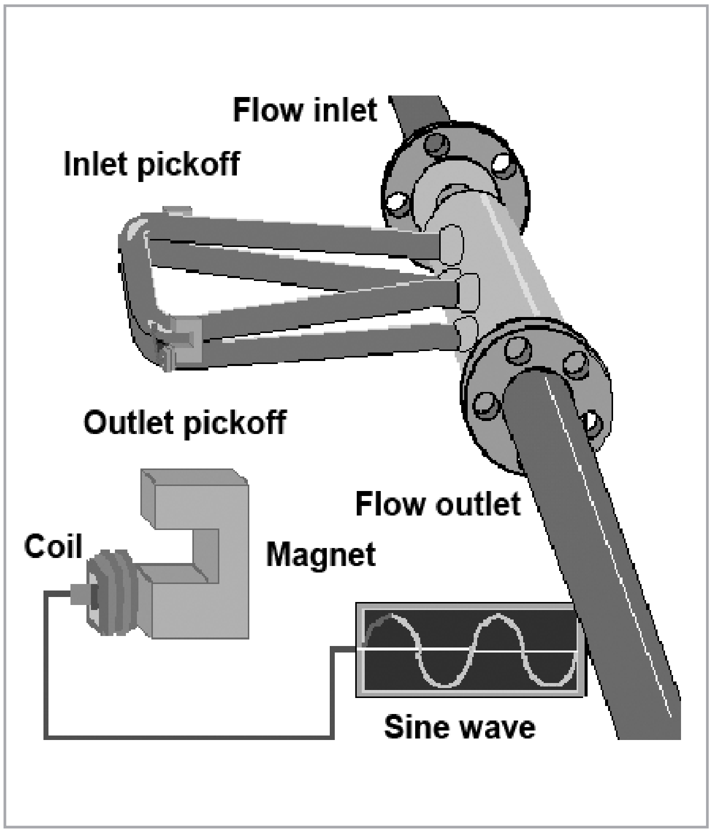

Figure 1: Coriolis Principle

Being the only flow meter that gives readings in mass per unit time for gas application, Coriolis Flow Meter is a very expensive flow meter compare to other flow meter such as volumetric flow meter, which are widely available in the market. Compare to other flow meters, the difference on the unit price is very significant. Therefore, the objective of the present research is to develop an alternative, cheap and efficient metering system to eliminate dependency on Coriolis flow meter.

2.0 MATERIALS AND METHOD

As an alternative flow meter to replace Coriolis, volumetric flow meter was found to be very attractive because of its lower price. However, volumetric flow meter gives reading in volume/time and this unit does not comply with the natural gas custody transfer regulations. To compensate for this, a conversion tool based on an *equation of state* (EOS) was developed to calculate mass flowrate of natural gas using volumetric flow meter, temperature and pressure data.

2.1 Equation of State (EOS)

An *equation of state* (EOS) [9] is a formula describing the interrelation between various macroscopically measurable properties of a system. For physical states of matter, equation of state usually relates the thermodynamic variables of pressure, temperature, volume and number of moles of material. The simplest *EOS* is the ideal gas law, which is given by

$$P\,V = n\,R\,T \tag{1}$$

where P is pressure, V is volume, n is number of moles, R is the universal gas constant and T is temperature. All substances behave according to this simple equation at sufficiently high specific volume (low density). This is because, at extremely low density, the individual molecules are essentially "point particles", occupying zero volume and never colliding with one another [10].

2.2 Development of the Conversion Model

In engineering applications, which are most often at atmospheric pressure or higher, no fluid is truly an ideal gas. However in many cases the assumption is within a few percent to be exact. Real gas laws try to predict the true behavior of a gas better than the ideal gas law by putting in terms to represent attractions and repulsions between molecules. These laws have been determined empirically, based on a conceptual model of molecular interactions or derived from statistical mechanics. The *Soave-Redlich-Kwong* (SRK) equation by Soave [11] was the first modification of the simple *Redlich-Kwong* (RK) equation where the parameter a, was made temperature dependent in such a way that the vapour pressure curve could be reproduced well.

The *Peng-Robinson* (PR) equation [12] is the most widely used equation in chemical engineering thermodynamics and modified by several researchers. Stryjek *et al*. [13] had proposed new alpha functions by introducing a new temperature dependence of the parameter $a(T)$ known as *Peng-Robinson-Stryjek-Vera* (PRSV) equation. It is known to give slightly better predications of liquid densities than the *SRK*. The *Lee-Kesler-Plocker* (LKP) equation is an accurate general method for non-polar substances and mixtures. Plocker *et al*. [14] applied the *Lee-Kesler* (LK) equation to mixtures, which itself was modified from the *Benedict-Webb-Rubin* (BWR) equation.

The *Zudkevitch Joffee* (ZJ) model [15] is a modification of the *RK* equation. This model has been enhanced for better prediction of vapour liquid equilibrium for hydrocarbon systems, and systems containing H_2. The major advantage of this model over the previous version of the *RK* equation is the improved capability of predicting pure component equilibrium, and the simplification of the method for determining the required coefficients for the equation. The *Kabadi-Danner model* (KD) [16] is a modification of the original *SRK* equation, enhanced to improve the vapour-liquid-liquid equilibrium calculations for H_2O-hydrocarbon systems, particularly in the dilute regions. The model is an improvement over previous attempts that were limited in the region of validity. The modification is based on an asymmetric mixing rule, whereby the interaction in the water phase (with its strong H_2 bonding) is calculated based on both the interaction between the hydrocarbons and the H_2O, and on the perturbation by hydrocarbon on the H_2O-H_2O interaction (due to its structure). In the following section, Table 1 summarizes the applicability of all models.

Table 1: Applicability of model

Model	Origins of model	Applicability of model
Soave-Redlich-Kwong	Redlich-Kwong	- Vapour pressure curve could be reproduced well
Peng-Robinson	-	- widely used in engineering thermodynamics
Peng-Robinson-Stryjek-Vera	Peng-Robinson	- Give better predications of liquid densities
Lee-Kesler-Plocker	Benedict-Webb-Rubin	- accurate method for non-polar substances and mixtures
Zudkevitch Joffee	Redlich-Kwong	- better prediction of vapour liquid equilibrium
Kabadi-Danner	Soave-Redlich-Kwong	- improve vapour-liquid-liquid equilibrium calculations

2.3 Application of EOS in Mass Flowrate Determination

EOS can be used to predict properties of mixtures ranging from well-defined light hydrocarbon systems to complex oil mixtures and highly non-ideal (non-electrolyte) chemical systems. Enhanced *EOS* such as *PR* and *PRSV* can be used for rigorous treatment of hydrocarbon systems; semi empirical and vapour pressure models for the heavier hydrocarbon systems; steam correlations for accurate steam property predictions; and activity coefficient models for chemical systems. In the following section, Table 2 lists some typical systems and recommended correlations.

Table 2: Recommended EOS for various applications

Type of System	Recommended Equations	Reference
Sour Gas	*PR*	Li and Guo [18]
Hydrocarbon with Hydrogen Sulfide and Carbon Dioxide	*SRK* *BWR*	Huron *et al*. [19] Evelein and Moore [20] Orye [21]
Carbon Dioxide and Chlorodiflouromethane Mixtures	*PR*	Lee *et al*. [22]
Non-aqueous Binary Mixtures	*SRK, PR, PRSV*	Lee and Lee [23]
Pure Alkanes, Ethers and Their Mixtures	*GCEOS*	Hofman *et al*. [24]
Oil Extraction Process	*ZJ, SRK*	Boss *et al*. [25]

From the table, it is shown that *EOS* is widely used in hydrocarbon system including natural gas. Radhakrishnan *et al*. [17] has conducted a study to compare all the *EOS* equations for measuring mass flowrate of natural gas using *NGV* refueling test rig located at *Universiti Teknologi Petronas* (UTP). By comparing results with Coriolis measurement, it was found that Peng Robinson was the most accurate equation and had been identified to be the *EOS* that could represent for high-pressure natural gas system. Thus, Peng Robinson was selected as *EOS* equation for the conversion purpose whilst the same test rig is used in this research.

2.4 Experimental Procedure

Two distinctive methods are used in determining the mass flowrate of natural gas passing through the measurement device: Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method. Data such as volumetric flowrate, pressure and temperature obtained from the test rig are used together with pre-identified *EOS i.e.*, Peng-Robinson and will be assessed using both methods in order to identify which method will be most reliable to be used.

Three dynamic experiments were also conducted. The difference between experiments is owed to the pre-determined experimental conditions such as the initial pressure of storage tanks and the initial pressure of vehicle or receiver tank to be refueled. For all experiments, three banks of storage tanks containing natural gas at same pressure *i.e.*, 3600 psig are used to provide the source of gas for refueling the vehicle tank up to a pressure of 3000 psig. The purpose of using three different banks is to enable for refueling to take place from one bank to another thus avoiding equal deterioration of pressure in all the storage tanks. It is essential to do so in order to ensure sufficient pressure drive is available from the storage tanks to continue refueling the natural gas to the vehicle tank up to the 3000 psig requirement. An automatic switching mechanism was installed to control the subsequent switch over from one bank to another. Dynamic experiment in this project is defined as experiment that is conducted continuously, meaning natural gas is dispensed continuously into the vehicle tank and experimental data are collected for every single second during the refueling. Data obtained from each set of experiment is analyzed using the two alternative measurement methods as described earlier in the paper. Results of analysis are presented in the following section.

In the Dynamic Mass Flowrate Method, the density of natural gas is assumed to be constant and the v variable in the *EOS* represents the molar volume of natural gas. Using this method, the algorithm will straight away provide the dynamic mass flowrate of natural gas dispensed using the experimental volumetric flowrate, temperature and pressure data. The first step in Dynamic Mass Density Method is to manipulate the original Peng-Robinson *EOS* to include mass term in the equation. The equations below are used in introducing the mass term;

$$v = \frac{V}{n} \tag{2}$$

$$n = \frac{m}{MW} \tag{3}$$

where,
v = molar volume (m^3/mol)
V = volume of tank (m^3)
n = number of mol of natural gas inside the vehicle tank (kmol)
m = mass of natural gas inside vehicle tank (kg)
MW = molecular weight of natural gas (kg/kmol)

With the substitution, the following equation is obtained;

$$\mathrm{P} = \frac{RT}{\frac{V\,(MW)}{m}} - \frac{a\alpha}{\frac{V\,(MW)}{m} - b\left(\frac{V\,(MW)}{m}\right)^2 + 2b\left(\frac{V\,(MW)}{m}\right) - b^2} \tag{4}$$

Since the concern is to obtain the mass flowrate instead of mass of natural gas inside the vehicle tank, the volumetric and mass flowrate terms is introduced to substitute the volume of tank and the mass of natural gas inside the tank and this is shown in the following equation;

$$\mathrm{P} = \frac{RT}{\frac{\dot{V}\,(MW)}{\dot{m}}} - \frac{a\alpha}{\frac{\dot{V}\,(MW)}{\dot{m}} - \mathrm{b}\left(\frac{\dot{V}\,(MW)}{\dot{m}}\right)^2 + 2b\left(\frac{\dot{V}\,(MW)}{\dot{m}}\right)} \tag{5}$$

where,
$\dot{V}$ = volumetric flowrate (m^3/min)
$\dot{m}$ = mass flowrate (kg/min)

The equation is then arranged into a polynomial form below so that the root of the equation will represent the mass flowrate of natural gas.

$$(Pb^3 + RTb^2 - ab\alpha)\dot{m}^3 - (a\alpha - 3Pb^2 - 2RTb)\dot{V}(MW))\dot{m}^2 + (Pb - RT)\,(\dot{V}(MW))^2\dot{m} - P(\dot{V}(MW))^3 = 0 \tag{6}$$

The next step is the computation of the mass flowrate of natural gas. Since it is impossible to obtain the mass flowrate by means of manual calculation, the MATLAB software is employed and utilising the root function, the mass flowrate of natural gas could be obtained.

In the Dynamic Density Flowrate Method, the v variable in the *EOS* represents the specific volume of natural gas hence the specific gas constant is used rather than the universal gas constant. Using this approach, the algorithm is arranged in such a way that it will provide the dynamic density of natural gas flowing through the measurement device and the mass flowrate of natural gas will be the product of the density and the volumetric flowrate given by the measurement device. The original *EOS* is manipulated to include density term in the equation. The equation below is used in introducing the density term;

$$v = \frac{1}{\rho} \tag{7}$$

where,
v = specific volume (m^3/kg)
ρ = density of natural gas (kg/m^3)

Thus, the following equation will be obtained;

$$\rho = \frac{RT}{v - b} - \frac{a\alpha}{v^2 + 2bv - b^2} \tag{8}$$

The equation is then arranged into a polynomial form below so that the root of the equation will represent the density of natural gas.

$$(Pb^3 + b^2RT - ab\alpha)\,\rho^3 + (3Pb^2 + 2bRT - a\alpha)\rho^2 + (Pb - RT)\rho + P = 0 \tag{9}$$

The MATLAB program is once again employed to solve for the root of the above equation, which represents the density of natural gas. The mass flowrate of natural gas dispensed into vehicle tank is the product of the dynamic density computed using the *EOS* and the volumetric flowrate measured by the alternative flow meter. For both methods, profiles of calculated mass flowrates using Peng Robinson equation and volumetric data are compared with actual mass flowrate directly measured by Coriolis flow meter to identify the deviation extent between them.

3.0 RESULTS AND DISCUSSIONS

Experiment 1 was conducted under automatic sequencing mode with initial storage pressure of 3600 psig for all three banks and refueling was done to a receiver tank with initial storage pressure less than 20 psig. The analysis using the Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method had produced mass flowrate result that was presented in Figures 2 and 3 respectively. Each of the figures represents calculated mass flowrate obtained from both EOS conversions respectively which was also compared with mass flowrate data obtained from actual Coriolis meter (*please refer graph legend*). From Figures 2 and 3 again, it was observed that the calculated mass flowrate followed the trend of actual Coriolis flowmeter. For experiment 1, the average error for Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method compared to Coriolis were 6.755% and 4.973%, respectively. Average error was defined as error of mass flowrate between the developed method and Coriolis measurement starting from initial pressure until receiver pressure reaches about 3000 psig.

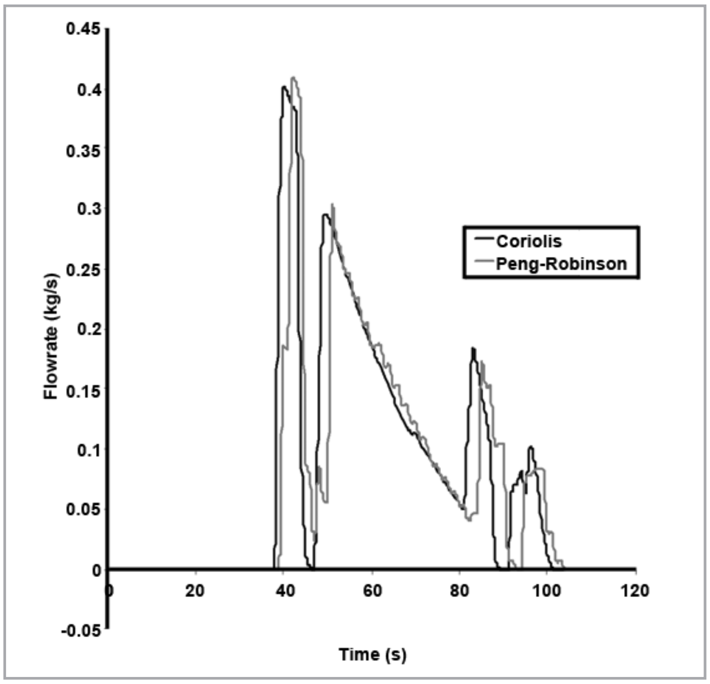

Figure 2: Mass flowrate for experiment 1 using dynamic mass flowrate method

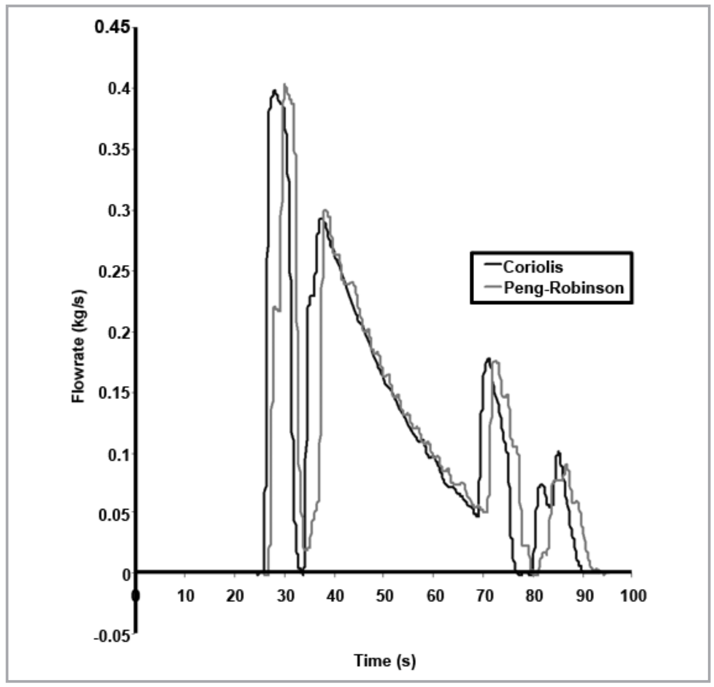

Figure 3: Mass flowrate for experiment 1 using dynamic density flowrate method

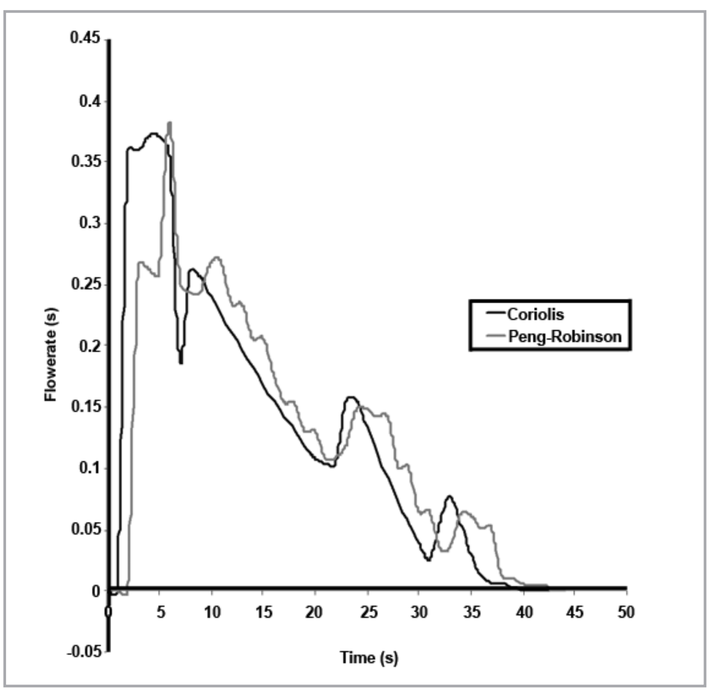

Figure 4: Mass flowrate for experiment 2 using dynamic mass flowrate method

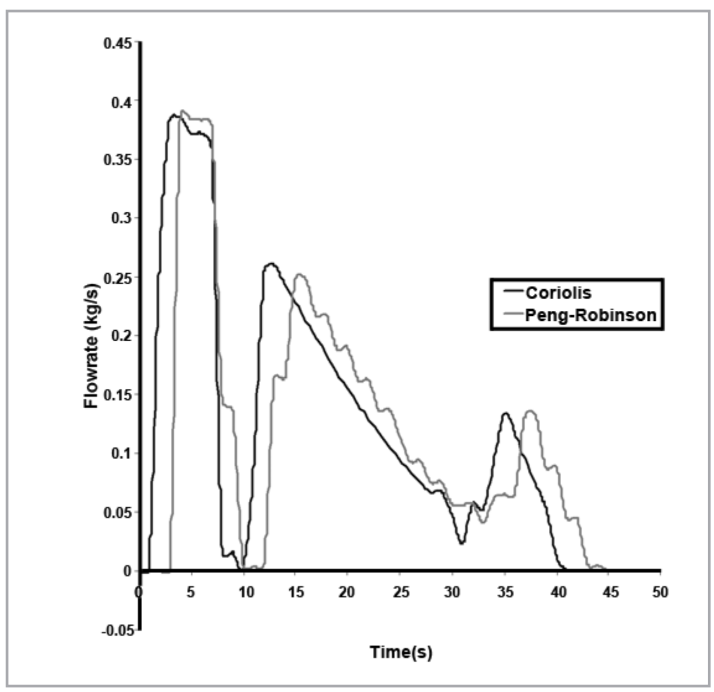

Figure 5: Mass flowrate for experiment 2 using dynamic density flowrate method

Experiment 2 was conducted with initial storage pressure of 3600 psig for all the 3 banks and receiver's initial pressure was about 1000 psig. The result of mass flowrates obtained using the Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method was shown in Figures 4 and 5, respectively. From Figures 4 and 5 again, it was observed that the mass flowrate obtained using the *EOS* conversion measurement followed the trend of the Coriolis plot. However, there was still a reasonably big deviation from the reference. For experiment 2, the average error for Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method compared to Coriolis were 5.889% and 0.791%, respectively.

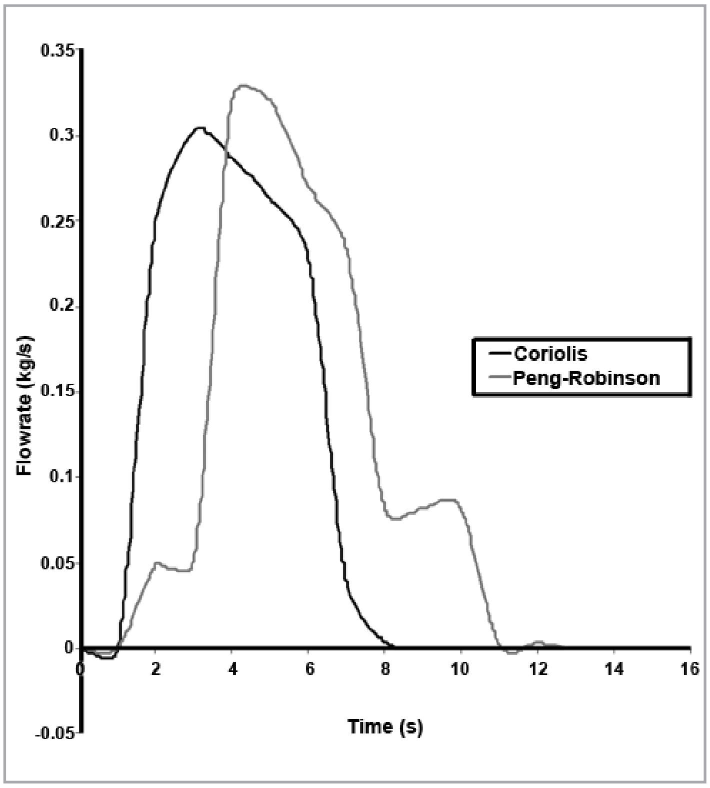

Figure 6: Mass flowrate for experiment 3 using dynamic mass flowrate method

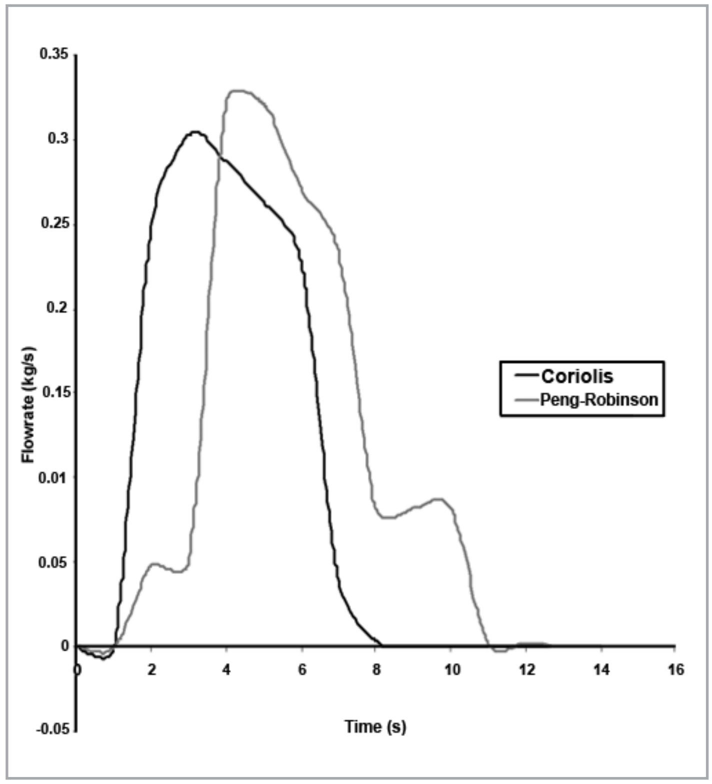

Figure 7: Mass flowrate for experiment 3 using dynamic density flowrate method

Experiment 3 was conducted with initial storage pressure of 3600 psig for all the 3 banks and receiver's initial pressure was about 2000 psig. The results obtained using the Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method was shown in Figures 6 and 7, respectively. From Figures 6 and 7 again, it was observed that the mass flowrates obtained using the developed *EOS* metering system followed the trend of the Coriolis plot. For experiment 3, the average error for Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method compared to Coriolis were 8.995% and 2.533% respectively.

Even though the natural gas was transferred from only three storage banks, it was clearly observed that there were four maximum peaks in all graphs. The first peak was the turn out of the initialisation of flow as stated in the process description, while the subsequent three peaks were due to the sudden flow increase of natural gas as a result of switching from one bank to another. An error analysis was done to detect which methods produced minimal error compared to Coriolis. Tables 3 and 4 show the result of error analysis.

Table 3: Error analysis for dynamic mass flowrate method

Experiment	Method	Coriolis (kg)	EOS (kg)	Error (%)
1	Mass	8.734	8.144	6.755
2	Mass	5.791	5.450	5.889
3	Mass	1.373	1.496	8.995
Average Error				7.213

Table 4: Error analysis for dynamic density flowrate method

Experiment	Method	Coriolis (kg)	EOS (kg)	Error (%)
1	Density	8.760	8.324	4.973
2	Density	5.700	5.655	0.791
3	Density	1.411	1.446	2.533
Average Error				2.766

From the error analysis, it was found that Dynamic Density Flowrate Method had produced smaller average error compared to Dynamic Mass Flowrate Method which was 2.766% compared to 7.213% respectively.

5.0 CONCLUSIONS

In this research, two distinctive methods were presented to be used as conversion tool in determining the mass flowrate of natural gas: Dynamic Mass Flowrate Method and Dynamic Density Flowrate Method. However, when both methods were compared with actual measurement using Coriolis flowmeter, it was found that Dynamic Density Flowrate Method had produced minimal average error compared to Dynamic Mass Flowrate Method. From the results obtained and analysis performed, it was found that the average error between Dynamic Density Flowrate Method and data measured by Coriolis flow meter was about 2.766%. Thus, Dynamic Density Flowrate Method was verified as the suitable conversion tool to be used as *EOS* metering system for converting volumetric to mass flowrate of natural gas. From here, it could be said that the research objective to develop an alternative metering system which offer an efficient and lower cost method for measuring mass flowrate in *NGV* refueling measurement has been successfully achieved. ■

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PROFILES

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