MODELING THE FAST FILL PROCESS IN NATURAL GAS VEHICLE STORAGE CYLINDERS

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INTRODUCTION

The on-board storage capacity of natural gas vehicles (NGVs) is a critical issue to the wide spread marketing of these alternate fueled vehicles. Underfilling of NGV cylinders, during fast fill (<5 min.) charging operations, can occur at fueling stations, at ambient temperatures greater than 50°F or 60°F. The resulting reduced driving range of the vehicle is a serious obstacle which the gas industry is striving to overcome, without resorting to unnecessarily high fueling station pressures, or by applying extensive overpressurization of the cylinder during the fueling operation. Undercharged storage cylinders are a result of the elevated temperature which occurs in the NGV storage cylinder, due to compression and other processes which have not, to the author's knowledge, been analyzed and documented to date.

This paper presents a model and solution methodology which quantifies the cylinder undercharging phenomena which occurs during rapid (<5 min.) fueling. The effects of heat transfer from the cylinder gas to its constraining walls and ambient are considered in the model analysis. The ramifications of the results on fueling station and cylinder designs are discussed. Suggestions are made for controlled experimental programs to verify the theoretical results, and for fueling station design studies which could minimize or eliminate cylinder underfilling.

ANALYSIS

MODEL ASSUMPTIONS

The following assumptions are made in the development of a mathematical model for fast charging natural gas cylinders.

1. The NGV cylinder is constant volume; there is negligible change in potential energy of the gas from the supply to the cylinder, and the kinetic energy of the cylinder gas is negligible. The pressure and temperature of the cylinder gas are not spatially dependent, i.e. quasi-steady perfect mixing occurs in the cylinder.
2. The mass flow, into the cylinder volume, is considered to be an isenthalpic expansion through an orifice.
3. The gas supply volume is infinite, with supply pressure and temperature remaining constant.
4. Heat transfer, from the cylinder control volume, is described by convective type heat flow to a lumped mass, cylinder wall. The cylinder wall temperature is not spatially dependent. Heat loss from the cylinder wall to the ambient is considered to be natural convection.

MODEL EQUATIONS

In applying the above assumptions to the natural gas storage cylinder charging model, shown in Fig. 1, one notes there are four basic dependent dynamic variables; the cylinder gas pressure, gas temperature, and mass of gas, and the lumped cylinder wall temperature. Four independent physical concepts are therefore needed for a dynamic solution.

The first physical concept applied is the dynamic energy equation for the NGV cylinder control volume, given in Equation (1). Note that each unit of supply gas, which enters the cylinder, has enthalpy, i.e. not only the internal energy of the gas in the supply, but also the supply "pv" work, associated with its flow. Note also that the gas in the cylinder volume contains only internal energy. One of the reasons behind the temperature rise of the gas in the cylinder, during a fast fill operation, lies in this conversion of enthalpy into internal energy.

The conservation of mass is the second physical concept utilized and is given in Equation (2). The supporting equations describing the assumed single orifice type flow rate are given in Equations (4) through (8). For adiabatic cylinder charging solutions of the set of modeled equations, the characteristics of the orifice, i.e. its area, rate of fill, or pressure ratio dependency will not affect the end temperature state in the cylinder, after a fill process to a given pressure. With heat transfer considered during cylinder charging, the flow rate characteristics of the orifice do influence the dynamic rates of heat exchange between the cylinder gas and cylinder wall, which in turn affects the end state cylinder gas temperature.

In this analysis, real natural gas properties are utilized to determine the property variables needed in the dynamic solution, i.e. enthalpy, internal energy, density, etc. These properties are obtained from subroutines which operate on pressure and temperature dependent tabulated results from the NIST computer program "STRAPP". The applicable equation of state, which provides a third physical concept, is given in Equation (3), or in its differential form, Equation (3a).

In deriving the basic differential equation set, reductions of Equations (1), (2), and (3) were used to solve for the NGV cylinder temperature, mass, and pressure respectively. The fourth dependent variable, the cylinder lumped mass wall temperature, is determined by the differential equation (10), after applying the supporting equations for the heat transfer into and out of the lumped mass wall, given in Equations (9) and (10) respectively. Fig. 2 shows a schematic of the cylinder wall heat transfer model.

SOLUTION PROCEDURE

The above described set of differential equations were numerically solved using the Runge-Kutta fourth order method, in a FORTRAN based computer program. Dynamic solutions for the cylinder gas pressure, temperature, and mass, and for the lumped cylinder wall temperature are output in the program together with integrated values for total heat transferred to and from the cylinder walls. Solutions end when the NGV cylinder pressure reaches a user-input pressure level.

MODEL RESULTS

TRANSIENT SOLUTIONS

Numerical solutions were developed using a mean U.S. natural gas composition whose components, by molar percentages are: Methane-92.87%, Ethane-3.34%, Nitrogen-2.07%, Carbon Dioxide-0.78%, Propane-0.63%, and less than 0.1% of I-Butane, N-Butane, I-Pentane, N-Pentane, and N-Hexane.

Examples of the dynamic pressure and temperature profiles in a 10" diameter, 50" long, NGV cylinder, during an adiabatic fill, are shown in Figures 3 and 4 respectively. In these results, the infinite supply gas conditions were 3000 psia and 70°F, while the initial cylinder pressure utilized was varied between 100 psia, simulating a nearly empty NGV cylinder, to 2500 psia, which could describe the topping off of a vehicle storage tank. The orifice size for the charging process was chosen so that the cylinder would fill to within 10 psi of the 3000 psia supply level in about 4 minutes, when starting from a nearly empty, 100 psia cylinder. In actual fueling operations, from 50 to 100 psi minimum pressure difference may be necessary between the fueling station cascade supply and the cylinder, to accommodate the station metering requirements or other piping or filtration flow impedances.

Note, from Fig. 4, that the cylinder gas temperature dips significantly during the early stages of charging a nearly empty cylinder, before rising to a final level of about 145°F. Note also that when charging a nearly full cylinder, the gas temperature profile is monotonic, reaching successively lower final values, as the initial pressure of the cylinder gas increases. The reason for the dip in temperature, in the early part of the filling of a nearly empty cylinder, lies in the

Joule-Thompson cooling effect, which the gas undergoes in the isenthalpic expansion through the orifice, from the 3000 psia supply pressure to the initially low 100 psia cylinder pressure. This cold gas mixes with and compresses the gas originally in the tank, with the result that the combined mixed gas temperature initially reduces. When the compression and conversion of supply enthalpy energy to cylinder internal energy overcomes the Joule-Thompson cooling effect, which becomes smaller as the cylinder pressure rises, the mixed gas temperature in the cylinder begins to rise. If the initial gas pressure in the cylinder is relatively high, the Joule-Thompson cooling effect is smaller, and does not, at any time, overcome the supply enthalpy conversion to cylinder internal energy. In this case, the cylinder gas temperature is seen to rise monotonically.

CYLINDER MASS FILL RATIOS

The charge parameter, which is directly related to the range of the NGV, is the cylinder "fill ratio", defined as the charged cylinder mass divided by the mass which the cylinder could hold at the rating condition of 70°F ambient and a pressure of 3000 psia. Fig. 5 shows how the mass fill ratio varies with initial cylinder pressure and supply pressure, for two values of the cylinder inside heat transfer coefficient. The adiabatic charge case corresponds to $H_{cyl}=0$, while the $H_{cyl}=5$ Btu/(hr-sqft-F) results apply to a heat transfer coefficient which is 10 times the assumed ambient side natural convection transfer coefficient of $H_{amb}=0.5$ Btu/(hr-sqft-F).

The inside cylinder heat transfer coefficient is difficult to estimate, since the gas flow into the cylinder is highly dynamic, and depends on numerous fluid, orifice, and cylinder parameters which are themselves rapidly changing in the charging process. Experiments are suggested which might lead to the measurement of average values which could then be used for this coefficient.

As seen in Fig. 5, the consideration of the heat transfer to the cylinder wall, with the assumed $H_{cyl}=5$ Btu/(hr-sqft-F) value, provides little change in the mass fill ratio. With initial cylinder pressures up to about 1000 psia, the model results show that a NGV fast fill operation will only load the cylinder to about 80% of the rated mass level. Thus, unless H_{cyl} is found experimentally to average much larger than 5 Btu/(hr-sqft-F), little help can be expected from the heat transfer to the cylinder wall in alleviating the cylinder underfilling situation.

CYLINDER CHARGING REQUIREMENTS

NGV fueling stations must take into account at least ambient conditions when recharging cylinders to maximize the range of the vehicle, while at the same time avoid overcharging, with its possible safety problems.

Fig. 6 plots, for the adiabatic charge case, how the charged pressure in the NGV cylinder would vary with ambient temperature, to achieve a fully charged mass condition, defined as the rated mass in the cylinder at 3000 psia and 70°F. Note the influence of the supply pressure is small in determining the required charged cylinder pressure. The cooled pressure curve reflects the effect of ambient temperature on the rated cylinder mass.

As an example, if the ambient were 70°F, to achieve a cooled cylinder pressure of 3000 psia, the cylinder would need to be fast charged to about 4000 psia, if the supply gas were at 5000 psia. If the ambient were 100°F, the cylinder would need to be charged to about 4600 psia, to achieve the rated mass level.

This dynamic overpressurization is a source of design difficulty for not only the NGV cylinder manufacturer, but also for the fueling station manufacturer and operator, since the fueling station compressor discharge and ground storage would need to be at least 5000 psia, to insure a fully charged cylinder at high ambients.

NOMENCLATURE

Parameters and Variables		Units
A	= area	in^2
C_d	= orifice discharge Coefficient	--
C_p	= specific heat at constant pressure	$Btu/(lb_m\text{-}^oR)$
C_v	= specific heat at constant volume	$Btu/(lb_m\text{-}^oR)$
d	= differential	--
f	= functional	--
g_c	= dimensionalizing factor	$(lb_m\text{-}in)/(lb_f\text{-}sec^2)$
h	= specific enthalpy	Btu/lb_m
H	= convective heat transfer coefficient	$Btu/(in^2\text{-}sec\text{-}^oR)$
k	= ratio of specific heats, C_p/C_v	--
M	= mass	lb_m
P	= pressure	$(lb_f/in^2)_{abs}$
Q	= heat transfer	Btu
R	= gas constant	$(in\text{-}lb_f)/lb_m\text{-}^oR)$
t	= time	sec
T	= temperature	^oR
u	= specific internal energy	Btu/lb_m
V	= volume	in^3
W	= orifice flow rate	lb_m/sec
Z	= compressibility factor	--

Subscripts

amb = ambient

cyl = cylinder

r = receiver cylinder

s = gas supply

w = cylinder wall

1 = orifice

EFFECTS OF COOLING THE SUPPLY GAS

One opportunity, to alleviate the need for creating and storing such high pressures in the fueling station, lies in the cooling of the supply gas, if a practical and cost effective way could be developed.

Fig. 7 shows the effects of cooling the supply gas, assumed to be at 4000 psia, to various temperature levels. As in Fig. 6, these results were created from the model for the adiabatic charge scenario. Note that by cooling the supply gas to 60°F, the required charged pressure, even at 100°F ambient, is reduced to about 3950 psia, to achieve a fully charged cylinder status.

RECOMMENDATIONS FOR FUTURE RESEARCH

Future research is recommended in three areas associated with the fast fill NGV problem. First, additional model development is needed to consider finite supply reservoirs, in a commonly used cascade group of three, which might be designed and controlled during the fast fill operation to reduce the temperature rise in the NGV cylinder. Second, experiments are proposed to support the model development, on well instrumented cylinders. Dynamic measurement of the mass entering the cylinder is needed to assure a proper model of gas flow rate profile. Experiments with the supply reservoir ambient at lower temperatures, relative to a cylinder located in a lab environment, would simulate the theoretically large supply gas cooling effect. Lastly, research and design studies are recommended to determine practical ways of cooling and storing the gas supply in the fueling station.

LIST OF EQUATIONS

Energy Balance

$$\frac{dQ_r}{dt} + W_1 h_s = \frac{d}{dt}\left(M_r u_r\right) \tag{1}$$

Conservation of Mass

$$\frac{dM_r}{dt} = W_1 \tag{2}$$

Equation of State

$$P_r V_r = R Z_r M_r T_r \tag{3}$$

in differential equation form, with V_r = constant

$$v_r \frac{dP_r}{dt} = R \frac{d}{dt}\left(Z_r M_r T_r\right) \tag{3a}$$

Orifice Flow Equation

$$W_1 = C C_{d_1} A_1 \frac{P_s}{\sqrt{T_s}} f\left(\frac{P_r}{P_s}\right) \tag{4}$$

where

$$C = \sqrt{\frac{g_c k}{R\left(\frac{k+1}{2}\right)^{\left(\frac{k+1}{k-1}\right)}}} \tag{5}$$

$$f\left(\frac{P_r}{P_s}\right) = 1 \text{ for } \frac{P_r}{P_s} \le \left(\frac{P_r}{P_s}\right)_{crit} \tag{6}$$

$$f\left(\frac{P_r}{P_s}\right) = \sqrt{\left(\frac{2}{k-1}\right)\left(\frac{k+1}{2}\right)^{\left(\frac{k+1}{k-1}\right)}}\left(\frac{P_r}{P_s}\right)^{\left(\frac{1}{k}\right)}\sqrt{1-\left(\frac{P_r}{P_s}\right)^{\left(\frac{k-1}{k}\right)}} \tag{7}$$

$$\text{for } \frac{P_r}{P_s} > \left(\frac{P_r}{P_s}\right)_{crit}$$

$$\left(\frac{P_r}{P_s}\right)_{crit} = \left(\frac{2}{k+1}\right)^{\left(\frac{k}{k-1}\right)} \tag{8}$$

Heat Flow Into Cylinder Wall

$$\frac{dQ_r}{dt} = -H_{cyl}A_{cyl}(T_r - T_w) \tag{9}$$

Heat Flow From Cylinder Wall to Ambient

$$\frac{dQ_{amb}}{dt} = H_{amb}A_{cyl}(T_w - T_{amb}) \tag{10}$$

Cylinder Wall Temperature

$$\frac{dT_w}{dt} = \frac{1}{M_w C_{p_w}}\left(\frac{dQ_w}{dt}\right) \tag{11}$$

$$\frac{dT_w}{dt} = \frac{1}{M_w C_{p_w}}\left(-\frac{dQ_r}{dt} - \frac{dQ_{amb}}{dt}\right) \tag{11a}$$

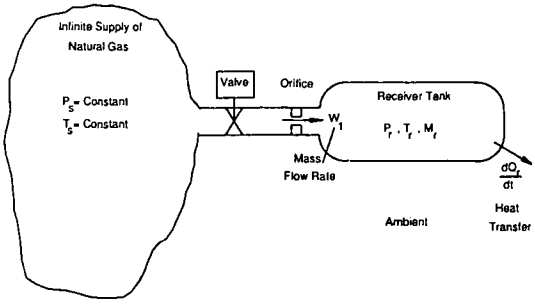

Fig. 1 Natural gas storage cylinder charging model

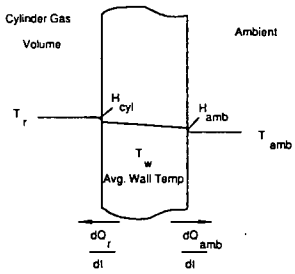

Fig. 2 Model of heat transfer through cylinder wall

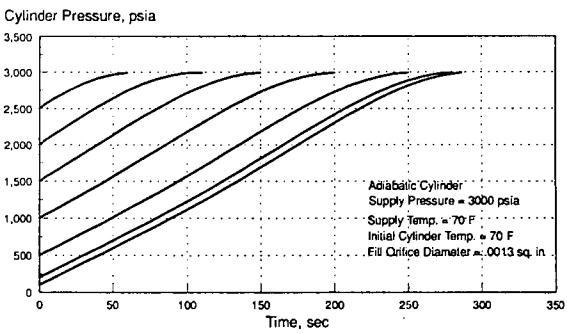

Fig. 3 Pressure in a 10"x50" Aluminum cylinder during a 3000 psia charge

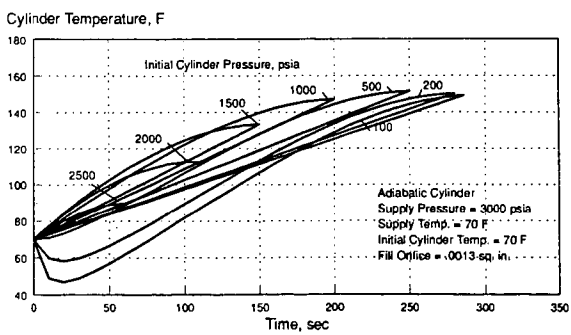

Fig. 4 Temperature in a 10"x50" Aluminum cylinder during a 3000 psia charge

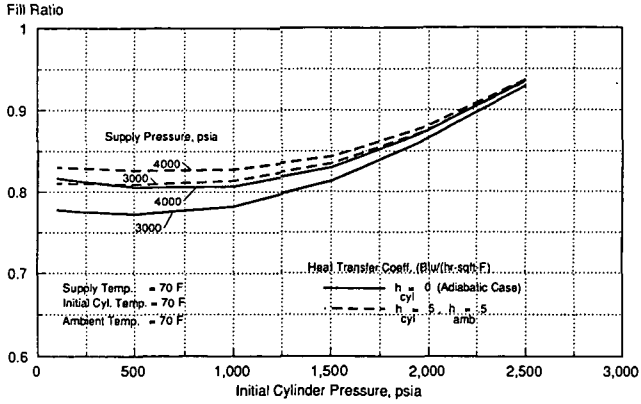

Fig. 5 Natural gas fill ratio in a 10"x50" Aluminum cylinder at the end of a 3000 psia charge

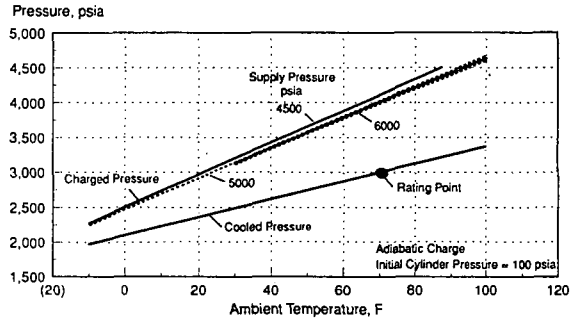

Fig. 6 Charged and cooled cylinder pressures for the rated charged mass, at 3000 psia and 70 F

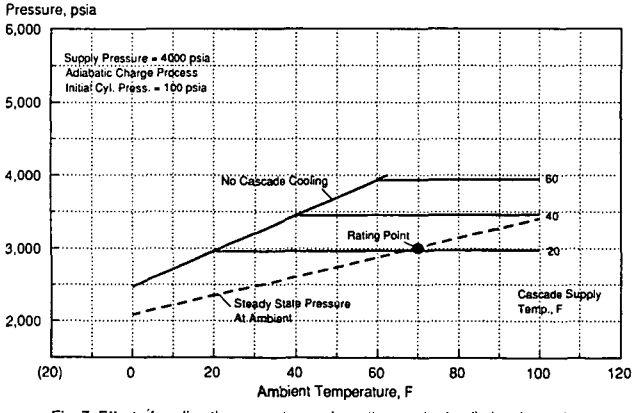

Fig. 7 Effect of cooling the cascade supply on the required cylinder charged pressure