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Research Paper

Dynamic simulation of liquefied petroleum gas vaporisation for burners

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HIGHLIGHTS

- A thermodynamic model is developed to investigate the vaporisation characteristics of LPG in a cylinder.
- Transient characteristics of LPG vaporisation are analysed under various conditions.
- The effects of various parameters on LPG vaporisation and the residues in LPG are analysed.
- A graphical procedure is proposed to determine the design value of Wobbe Index for burners.

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ABSTRACT

This study numerically describes the transient behaviours of liquefied petroleum gas (LPG) natural vaporisation in a cylinder using an experimentally validated model. The model can be applied to easily predict transient compositions and thermophysical properties during the vaporisation process under various conditions. A simple graphical design procedure is presented to determine the Wobbe Index and the corresponding composition as design references for gas burners to avoid incomplete combustions. The effects of initial composition, surrounding temperature and discharge rate of LPG on both the LPG natural vaporisation and the residue amount in the cylinder are simulated and investigated. The results demonstrate that the present work may serve as a useful tool to evaluate the LPG behaviours throughout the vaporisation, design or retrofit gas burners, and predict the unburned residue.

1. Introduction

Liquefied petroleum gas (LPG) is mainly composed of propane (C_3H_8) and *n*-butane (C_4H_{10}) with some propylene (C_3H_6), butylene (C_4H_8), and other minor compositions of hydrocarbons. LPG is in gaseous form at ambient temperatures and pressures. Due to a dramatic reduction in the volume after being liquefied, LPG is commonly stored and transported in liquid form in pressurised steel cylinders. This makes LPG a popular domestic fuel in rural and remote areas, even in some urban regions away from natural gas transmission networks [1]. For instance, Chinese total LPG consumption for householders was 21.73 million tons in 2014 [2].

The common way for domestic and commercial burners to use LPG is to supply liquid LPG in commercially available cylinders without thermal insulation and then to use it in gaseous form. The liquid-to-vapour phase change occurring within the cylinder is called spontaneous (or natural) vaporisation in which process the heat for

vaporisation comes from the liquid itself and/or from the surroundings and components with lower boiling points vaporise easier and earlier. The properties of both the liquid and the vapour vary continuously with the change in LPG compositions over time. The minimum inlet pressure of a gas regulator automatically modulates high-pressure gas to a safe pre-determined limit for gas burners, so the cylinder cannot be completely emptied and the remaining liquid is called as the residue. It means that if the vapour pressure in the cylinder is less than the required minimum value, the natural vaporisation process will be completed.

To estimate the physical properties of LPG and the residue amount, it is necessary to know the composition [3]. The chromatography method is usually applied to determine the composition of LPG after analysing its sample [4–7]. However, it is hard to adopt this method to continuously determine the composition that changes instantaneously through the vaporisation process. Some mathematical models were developed to predict the dynamic behaviours of LPG spontaneous

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Nomenclature

A_A	antoine parameter
a	coefficient in SRK equation
B_A	antoine parameter
b	coefficient in SRK equation
C_A	antoine parameter
C_p	specific heat ($\text{kJ kg}^{-1} \text{K}^{-1}$)
D	Inner Diameter (m)
e	ratio of moles of gaseous LPG to total moles of LPG
\hat{f}	fugacity (Pa)
H	height of liquid level (m)
H_T	height of cylinder (m)
K	phase equilibrium constant
k	overall heat transfer coefficient ($\text{kW m}^{-2} \text{K}^{-1}$)
M	molecular mass (kg mol^{-1})
m_g	mass of gaseous LPG (kg)
m_{go}	mass flow rate (i.e. discharge rate) (kg s^{-1})
m_l	mass of liquid LPG (kg)
P	pressure (Pa)
P_{sat}	saturation pressure (Pa)
Q	heat (kJ)
R	universal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
r	specific latent heat (kJ kg^{-1})
T	temperature (K)

t	time (s)
V	mole volume ($\text{m}^3 \text{mol}^{-1}$)
w	mass fraction (%)
x	mole fraction in liquid phase (%)
y	mole fraction in vapour phase (%)
Z	compressibility factor
z	total mole fraction (%)

Greek

ρ	density (kg m^{-3})
$\hat{\phi}$	fugacity coefficient
ω	acentric factor

Subscripts

0	standard state
c	critical point
Cy	cylinder
Env	surroundings
g	gaseous phase
i	component i
j	component j
l	liquid phase

vaporisation in the cylinder [3,8,9]. However, such models are typically valid for specific and rigorous assumptions. The LPG within the cylinder was assumed to be ideal [3,8,9]. Furthermore, Yan [8] assumed that the change in LPG composition did not alter the values of some thermodynamic properties and the ratio of the pressure to the temperature of LPG kept constant. Tian and Jiang [3] treated the mass fraction of each component as an equivalent of its mole fraction and assumed that the LPG temperature remained unchanged throughout the vaporisation [3]. These above mentioned assumptions are in conflict with the practical natural vaporisation and may cause some limitations of the models.

This work emphasises the need to account for the non-ideal behaviour of both the liquid and the vapour phases in the pressurized steel cylinder and the importance of variable physical properties in investigating the real LPG spontaneous vaporisation process. The main objective of this study is to present a comprehensive model and explore the detailed transient characteristics of LPG natural vaporisation process for gas burners, which can provide a basis for designing or retrofitting burners to get good combustion performance and predicting the residue amount. First, a dynamic model is established which prediction accuracy is validated by using the previous experimental data. Further, the transient behaviours of LPG vaporisation are obtained and analysed, with special emphasis on variation of combustion properties of vapour LPG. Finally, the effects of initial composition, surrounding temperature and discharge rate on the natural vaporisation and the residue amount are discussed based on the simulation results.

2. Model development**2.1. Description**

As shown in Fig. 1, when the user opens the reducing valve to use LPG, the vapour flows out. Then the vapour pressure in the cylinder reduces and the equilibrium no longer exists. The liquid LPG has to vaporise immediately to mitigate the drop in the pressure and to regain a vapour-liquid equilibrium (VLE) condition. Due to no temperature difference, the latent heat of vaporisation is only from the liquid itself at the beginning. The liquid temperature thus decreases, which generates the temperature difference between inside and outside of the cylinder.

The heat for vaporisation then comes from both the liquid and the surroundings.

2.2. Model assumptions

Five assumptions have been made concerning the simulation.

- The temperature is uniformly distributed in the cylinder and the vapour has the same temperature as the liquid.
- The cylinder wall and the LPG are in the same temperature.
- The cylinder's surrounding temperature is constant throughout the

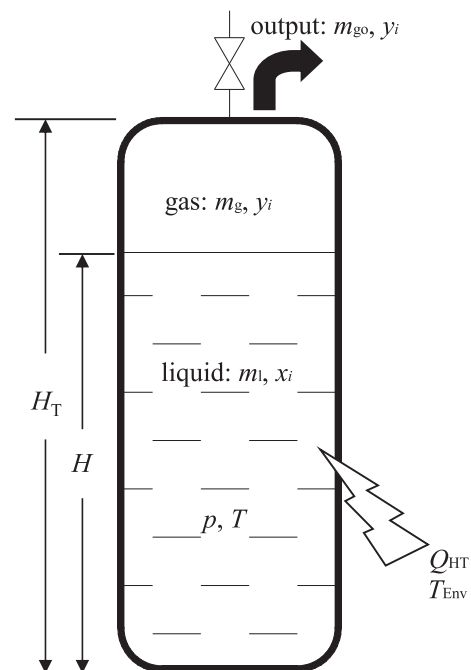


Fig. 1. Spontaneous vaporisation of LPG in a cylinder.

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