A Study on the Combustion Reaction and Control Algorithm Using Methane-Hydrogen Mixture Gas

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Abstracts

Since the Paris Agreement was adopted in 2015, the international community has proposed a basic roadmap to promote 2050 carbon neutrality. In the global boiler market, the roadmap was specified through fuel conversion by increasing the hydrogen content of LNG. Accordingly, research is being actively conducted to apply methane-hydrogen mixture gas to the existing boiler systems. However, various problems such as flashback and instability occur because the combustion characteristics of hydrogen are much different from those of methane. Therefore, it is necessary to secure the source technology of methane-hydrogen hybrid combustion system applicable to industrial sites. In this study, a Labview program was designed to secure various parameters generated by combustion of hybrid LNG and hydrogen mixture. The Labview program consists of a block diagram on which code can be designed and a front panel that serves as a user interface. Before coding, the complete combustion reaction equation was represented as an equation for x. Then, the algorithm was designed to perform repetitive calculations by constructing two consecutive loops. The hydrogen mixing ratio is derived from the first loop, and the oxygen concentration in the exhaust gas is derived from the second loop. Based on this algorithm, the block diagram was designed with the same corelations. By inputting the oxygen concentration value of the exhaust gas into the user interface, it is possible to predict the hydrogen mixing ratio and the air flow rate with respect to the corresponding input value.

1 Introduction

It has been recommended that global carbon neutrality be achieved to curb the average global temperature rise above 1.5°C compared to before industrialization [1]. The world began to declare carbon neutrality by 2050, and presented a basic roadmap to implement the goal. Recently, the government is promoting innovation in clean energy technologies in earnest to achieve carbon neutrality. In particular, hydrogen is a carbon-free fuel, which can reduce greenhouse gases while utilizing existing infrastructure such as boilers and generators [2].

As part of active research, Yitong Xie analyzed the effect of hydrogen mixing ratio and temperature on flame stability, and Li Guo derived the correlation between the hydrogen mixing ratio and the quenching distance of methane/hydrogen/air flame [3]. Tahsin BerkKyyma discussed the flashback dynamics of premixed methane-hydrogen-air laminar flames [4], and Xiaozhou Liu presented the temperature distribution of the flame according to the change in the hydrogen mixing ratio of the domestic swirl stove [5]. Xiuting Li explained the activation energy by dynamically analyzing methane/hydrogen mixtures combustion through the ReaxFF-MD simulation [6]. Researchers around the world are studying issues related to methane/hydrogen mixtures combustion, such as air ratio imbalance [7-13], flame stability and combustion speed. However, there is a lack of underlying data on prediction and control programs. It is important to develop a control system that can compensate for problems caused by the physical and chemical properties of hydrogen [14-15]. It will be different from the existing operating system, since the combustion characteristics of hydrogen are much different from those of CH4 (methane). In this study, an algorithm was developed, which can predict theoretical data of a hybrid combustor.

2 Experiment Setup and Methodology

In general, 1 mole of methane reacts completely with 2 moles of oxygen to form 1 mole of carbon dioxide and 2 moles of water. In the actual combustion reaction, oxygen gas is supplied with nitrogen gas because the air is made up of 21.0 mol% oxygen and 79.0 mol% nitrogen. Oxygen reacts with fuel while nitrogen does not participate in the reaction. Equation (1) shows a complete combustion reaction equation when methane is used as fuel. Equation (2) is a complete combustion reaction equation when 1 mole of methane and 1 mole of hydrogen are used as fuel.

$$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2 \quad (1)$$

$$CH_4+H_2+2.5(O_2+3.76N_2) \rightarrow CO_2+3H_2O + 9.4N_2 \quad (2)$$

In this study, it was designed based on the complete combustion reaction of methane-hydrogen fuel conversion. Equation (3) is a complete combustion reaction equation designed to be suitable for changes in the methane-hydrogen composition of the fuel. The methane mixing ratio and hydrogen mixing ratio of fuel were expressed as mole fractions as shown in Equations (4) and (5), so that the calculation could be facilitated [16].

$$xCH_4+(1-x)H_2+yO_2+3.76yN_2 \rightarrow xCO_2+zH_2O + 3.76yN_2 \quad (3)$$

$$\Delta CH_4 : x \quad (4)$$

$$\Delta H_2 : 1-x \quad (5)$$

The coefficients of the chemical equation can be obtained using the method of undetermined coefficients, since the number of atoms of the reactant and the product in Equation (3) is the same. The coefficients of Equation (3) were simply expressed as a function of x as shown in Equation (6), after erasing the unknowns, y and z.

$$xCH_4+(1-x)H_2+(1.5x + 0.5)O_2+3.76(1.5x + 0.5)N_2$$
$$\rightarrow xCO_2+(x + 1)H_2O + 3.76(1.5x + 0.5)N_2 \quad (6)$$

In the actual combustion reaction, excess air is supplied to the combustor and the concept of excess air quantity is applied to Equation (6). The excess air ratio k is set to a real number greater than 1, and Equation (7) is a complete combustion reaction equation when excess air is injected.

$$xCH_4 + (1 - x)H_2 + k(1.5x + 0.5)O_2 + 3.76k(1.5x + 0.5)N_2 \\ \rightarrow xCO_2 + (x + 1)H_2O + 3.76k(1.5x + 0.5)N_2 + (k - 1)(1.5x + 0.5)O_2 \quad (7)$$

Based on Equation (7), a program was constructed to control the fuel conversion system of methane-hydrogen mixture gases using oxygen concentration in exhaust gas. In this process, the National Instruments (NI) LabVIEW program, a graphics-based programming language, was used. Figure 1 shows problem-solving logic and a series of procedures through algorithms.

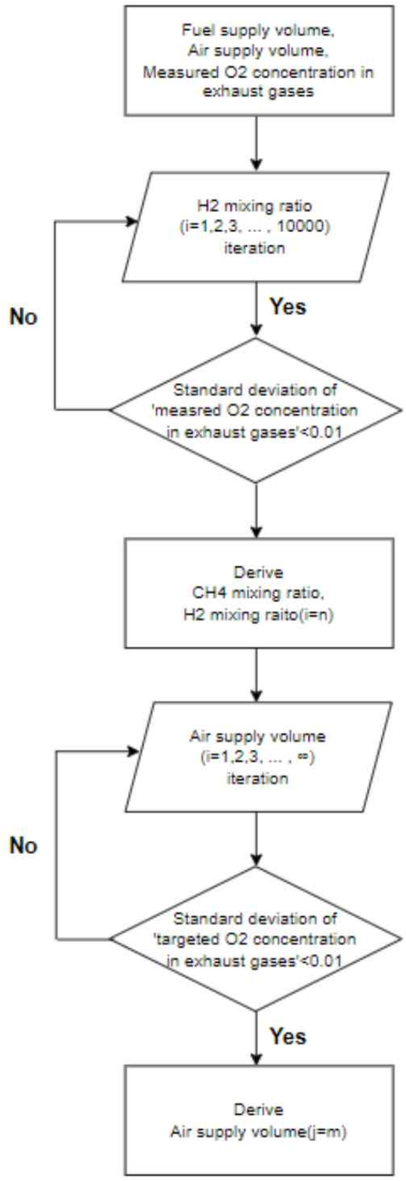

Figure 1: Program algorithm

In the LabVIEW program, two consecutive For-Loops were constructed, and the command is repeated N times of the integer input. They are designed to terminate the For-Loops when certain conditions are met. In the first For-loop, the hydrogen mixing ratio was set as a repeating terminal and was ordered to be repeated from 0 to 100 at 0.01 intervals. Starting with the calculation of the hydrogen mixing ratio i=1 (=0 vol.%), factors such as the methane mixing ratio, theoretical air volume, air ratio, high heat generation, low heat generation, and exhaust gas composition are sequentially calculated. Finally, the first For loop command ends when the standard deviation of 'calculated oxygen concentration in exhaust gas' and 'measured oxygen concentration in exhaust gas' becomes less than 0.01. The hydrogen mixing ratio derived from the first For loop is linked to the input value of the second For loop. After the algorithm of the first For-loop is stopped, the algorithm of the second For-loop is processed. In the second For-loop, the air supply volume was set as a repeating terminal and was ordered to be repeated from 0 to infinity at 0.01 intervals. Starting with the calculation of the air supply volume i=1(=0.0 vol.%), factors such as the theoretical air volume, air ratio, and oxygen concentration in the exhaust gas are sequentially calculated. If the standard deviation of ‘the calculated oxygen concentration in exhaust gas’ and ‘the targeted oxygen concentration in exhaust gas, 5.5 vol.%’ is greater than or equal to 0.01, the following calculation is performed at the hydrogen mixing ratio i=2 (=0.01 vol.%). The second For-loop command ends when the standard deviation of ‘the calculated oxygen concentration in the exhaust gas’ and ‘the targeted oxygen concentration in the exhaust gas’ becomes less than 0.01. Finally, the algorithm terminates when ‘the oxygen concentration in the exhaust gas’ is derived at the second For- loop end point.

3 Results and Discusssion

The algorithm in Figure 1 was introduced into the LabVIEW program. The LabVIEW program consists of a block diagram organized with wiring-type codes as shown in Figure 2 and Figure 3, and a user interface called front panel as shown in Figure 4. In the first For-loop, the hydrogen mixing ratio is finally derived based on ‘the measured oxygen concentration in exhaust gas’. In the second For-loop, the air supply volume is finally derived based on the oxygen concentration in exhaust gas. In the front panel, calculated data may be arranged and checked according to the code designed in the block diagram. This front panel is user-friendly because data can be checked in real time through input values, output values, and waveform chart, which are the main functions of this front panel. The oxygen concentration in the exhaust gas calculated in the first For loop and the second For loop was shown to be a wave function.

In the front panel, Input values include input fuel volume, air supply volume, and ‘measured oxygen concentration in the exhaust gas’, and Output (1) values include methane mixing ratio, hydrogen mixing ratio, and oxygen concentration in the exhaust gas. Connector values include input fuel volume, methane mixing ratio, hydrogen mixing ratio, and ‘targeted oxygen concentration in the exhaust gas’, and they are applied as input values for the second loop, which are shared between the two loops. Finally, air supply volume and the oxygen concentration in the exhaust gas are derived as Output (2) value of the second loop.

Figure 5 shows the theoretical air quantity when the oxygen concentration in the exhaust gas is controlled to be 5.5 vol.%. As the hydrogen mixing ratio increased, theoretical air quantity decreased from 214.0 Nm3/h to 53.0 Nm3/h, and the air ratio was constant at 1. On the other hand, the excess air quantity is shown in Figure 6 when the oxygen concentration in the exhaust gas is not controlled. As the hydrogen mixing ratio increased, the excess air quantity was constant at 297.0 Nm3/h, and the air ratio increased rapidly from 1.39 to 5.56. It is necessary to have a system to control the oxygen concentration in the exhaust gas to prevent a rapid increase in the amount of excess air. In this study, when the targeted oxygen concentration in exhaust gas is 5.5%, the air supply volume to be controlled is 244.0 Nm3/h. Under the standard temperature pressure (STP) condition, the values of output (1) and output (2) can be newly derived according to various input values of the front panel.

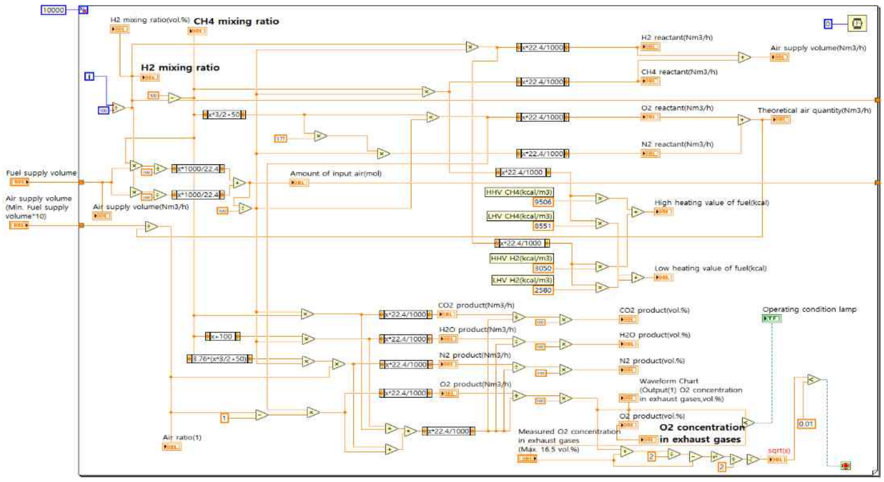

Figure 2: First loop block diagram

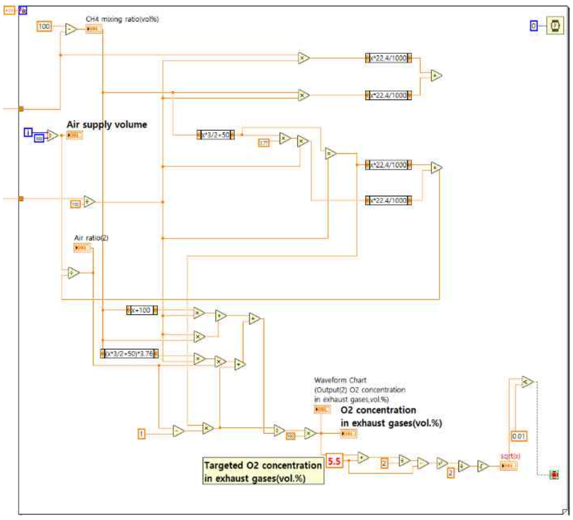

Figure 3: Second loop block diagram

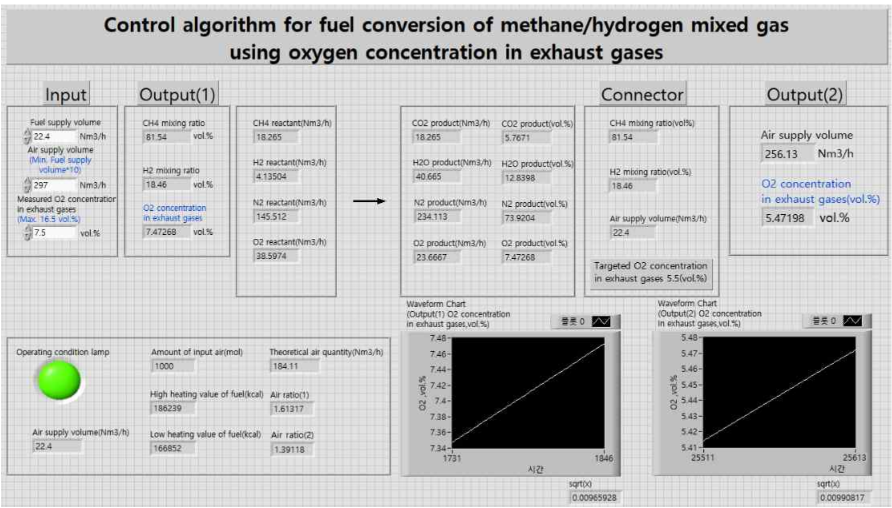

Figure 4: Front panel

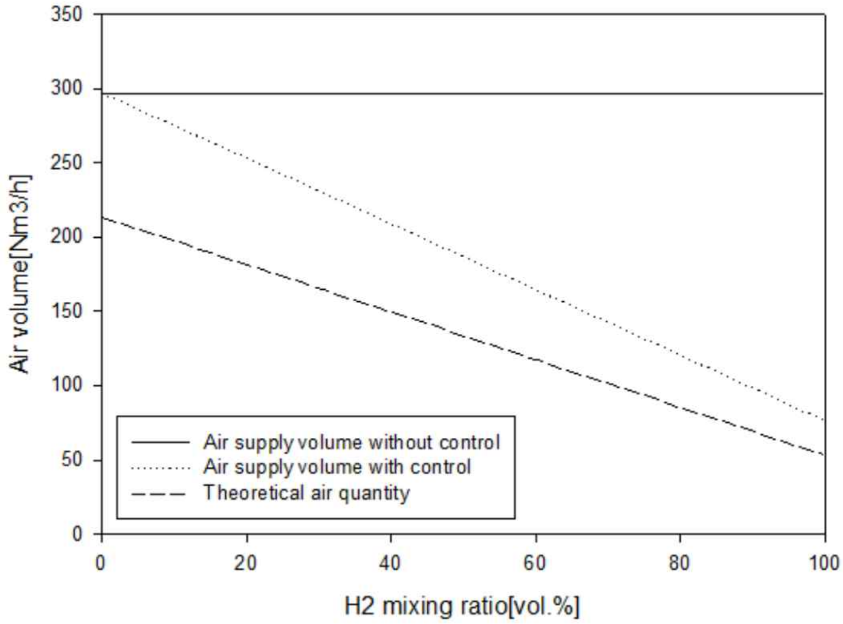

Figure 5: Comparison of air volume with and without control according to hydrogen mixing ratio

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