Preliminary investigation to the feasibility of chemical heat storage for saving the exhaust gas energy in a spark ignition engine

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Abstract

Heat storage has become more important because it utilizes the wasted energy to improve the overall efficiency of energy systems. This study was aimed to develop a chemical heat storage system using magnesium hydroxide (Mg(OH)₂) and its endothermic and exothermic reactions to recover the thermal energy of the exhaust gas in internal combustion engines. It was proposed that the reactor receives the thermal energy of exhaust gas in the dehydration of Mg(OH)₂ to become MgO and H₂O, and releases the stored energy in the hydration of MgO. To increase the thermal conductivity of pure Mg(OH)2 for enhancing the reactor's performance, the working material used, EM8 block, is the mixture of Mg(OH)2 and expanded graphite at a ratio of 8:1. Experiments were conducted on a 6-cylinder spark ignition engine (Toyota Aurion 2GR-FE 3.5L) at stoichiometric air/fuel ratios to estimate the amount of energy loss in the exhaust gas. Experimental data of exhaust gas temperature and volume ratios of exhaust gas constitutions were used to calculate the energy rates of each of the exhaust gas constituents and to estimate the reactor efficiency in the dehydration process. Results of the preliminary investigation show that the proposed chemical heat storage system may be feasible to recover approximately 5.8 % of the heat loss in the exhaust gas.

Introduction

In today's modern life, internal combustion (IC) engines are still widely used in many fields, such as transportation, construction or agricultural sectors. However, a significant amount of fuel energy is lost as wasted heat through exhaust gas and cooling systems in IC engines. Recovery of waste heat not only directly increases the engine overall thermal efficiency but also reduces the environment pollution. If a certain amount of exhaust gas heat could be recovered, the equivalent amount of primary fuel can be saved. As predicted, if 6% of the exhaust gas energy is converted to electric power, the same amount of electrical power will be released, and the fuel consumption could be reduced by 10% [1].

Energy storage is a method used to store energy wasted in a power system and use the stored energy when it is needed. It is usually divided into two groups: electrical and thermal [2]. Electrical energy storage includes electrochemical systems, kinetic energy storage systems and potential energy storage. Sensible, latent and chemical heat storages are classified as thermal energy storage. In the chemical heat storage technology, heat is stored in chemicals, so it has advantages as follows:

- Chemical energy storage has higher energy density than that with physical energy storage (sensible heat change or phase change) [3].
- Heat can be stored for a long period and with small heat loss. Chemicals are stored separately and in the ambient condition, so the heat lost to the environment is minimal.

The focus of this study is to apply the chemical heat storage technology to store a part of engine's wasted heat and uses it for heating purposes, such as defogging and heating or fuel heating for the cold-start process.

Chemical heat storage

Chemical heat storage technology uses the chemicals as heat storage materials. In the present study, it was proposed that the chemical $Mg(OH)_2$ be adopted. $Mg(OH)_2$ is an environmentally friendly material which exists abundantly in nature and its working temperature is in the range of the exhaust gas temperature at the engine exhaust port.

To store the heat of the exhaust gas, it was proposed that two main devices would be installed in the exhaust gas pathway, a reactor and a condenser/evaporator (condenser in the heat storage and evaporator in the heat output process).

In the heat storage mode, Magnesium hydroxide absorbs wasted heat of the exhaust gas and converts to magnesium oxide and water vapour in the dehydration of magnesium hydroxide in the reaction chamber, as shown in Figure 1.



Figure 1. The heat storage process.

During this chemical process, MgO is retained inside the reactor chamber, and the water vapour produced from the chemical reaction is moved into a condenser/evaporator to condensate. The equilibriums are expressed as follows:

$$Mg(OH)_2(s) + \Delta H_1 \rightarrow MgO(s) + H_2O(g)$$
 (1)

$$H_2O(g) \rightarrow H_2O(l) + \Delta H_2$$
 (2)

Magnesium oxide and water vapour produced from this process are stored separately in the ambient temperature so that they can be stored for a long time with small heat loss.



Figure 2. The heat output process.

In the heat output mode as shown in Figure 2, the water liquid in the evaporator is heated by a small heating tape to evaporate. Before heating, the water liquid is stored in the evaporator at low pressure and with small volume. Therefore, the energy required for evaporating (heating tape) the liquid water is very small compared with the stored exhaust gas energy. The water vapour will flow from the evaporator into the reaction chamber. The reaction takes place between the MgO and the water vapour, and heat energy will be released. The equilibriums are described as follows:

$$H_2O(l) + \Delta H_3 \rightarrow H_2O(g)$$
 (3)

(4)

$$MgO(s) + H_2O(g) \rightarrow Mg(OH)_2(s) + \Delta H_4$$

Estimation of the heat loss in the exhaust gas

To obtain the information needed to investigate the feasibility of chemical heat storage of engine exhaust gas energy, experiments were conducted on a 6-cylinder spark ignition Toyota Aurion engine. The major specifications of the engine are provided in table 1.

Parameters	Unit	Value
Number of cylinders		6
Number of strokes		4
Bore	mm	94
Stroke	mm	83.10
Displacement volume	сс	3456
Connecting red length	mm	147
Compression ration		10.8:1
Maximum power	kW	200@6200rpm
Maximum Torque	N.m	336@4700rpm

Table 1. Major specifications of the tested engine.

Experiments were conducted on the engine at the stoichiometric air-fuel ratio and 18 sample power conditions. The engine power is calculated based on the engine speed and torque. From measurement data, the exhaust gas temperature (was measured by a thermocouple installed at the exhaust port) and its components (were acquired by Horiba MEXA-584L gas analyser), heat loss is calculated by the summing the energy of components and is showed in figure 3.



Figure 3. The energy consumption.

As shown in figure 3, at the stoichiometric process ($\lambda = 1$), the average heat loss in exhaust gas is 31.93% of total energy and the aim of the current study is to cover part of the energy loss.

Estimation of the dehydration efficiency of the reactor

To store a part of the exhaust gas heat, a reactor is installed between the engine exhaust port and the catalytic converter. The experimental results (the temperature and components of the exhaust gas at the outlet of the engine exhaust port) were used in the initial design of the reactor and estimating the efficiency of the reactor in the dehydration or heat storage process in one hour working time.

Choosing chemical material

The material originally considered was magnesium hydroxide $(Mg(OH)_2)$.The thermal conductivity of the packed bed of $Mg(OH)_2$ pellets is within 0.15 – 0.16 W m⁻¹ K⁻¹ [4]. The decreased thermal conductivity of pure $Mg(OH)_2$ pellets will reduce the heat absorption capacity of chemical and thereby

decrease the efficiency of the reactor. To increase the heat transfer efficiency of chemical, Massimiliano suggested using a new material that was a combination of Mg(OH)₂ and expanded graphite with the mass mixing ratio 8:1 and in the block state (EM8 block) [4]. EM8 block was selected in the present study. As reported in [4], the advantages of this material compared with pure Mg(OH)₂ include:

- Higher thermal conductivity: The thermal conductivity of EM8 block is about ten times that of the pure Mg(OH)₂ pellets.
- Higher density: Compare with the density of the bed of pure Mg(OH)₂ pellets were randomly arranged in the reactor, the density of EM8 block is 1.6 times that of Mg(OH)₂ pellets. With higher density, the capacity of the energy storage system will be increased.
- Reduced void fraction of bed will enhance the contact between the thermochemical and the inner surface of the reactor and consequently improve the thermal conductivity of the reactor.

As investigated by Massimiliano[4], the volumetric heat storage of EM8 block and other compounds are showed in figure 4.



Figure 4. Comparison of volumetric heat storage capacity of pure Mg(OH)₂, EM8 in the pellets state and EM8 block [4].

As shown in figure 4, the heat storage capacity of EM8 block is 1.4 times that of pure $Mg(OH)_2$ and EM8-b (the combination of $Mg(OH)_2$ and expanded graphite in the mass mixing ratio is 8:1 and in the state of pellets) in one hour working time.

The volumetric heat storage capacity of EM8 block can be estimated using Eq. (5) [4]:

$$q_{d,v} = \frac{-\Delta H_r^0}{M_{M_g(OH)_2}} \Delta x_d r_{mix} \rho_{bed}$$
(5)

Where

 $q_{d,v}$ is the volumetric storage capacity (kJ/m³).

 $M_{Mg(OH)_2}$ is mole mass of Mg(OH)₂ (58.322 g/mol).

r_{mix} is the mass mixing ration.

 ρ_{bed} is the density of the packed bed ($\rho_{EM8 block}$ is 1.002 g/cm³).

 Δx_d is the mole reacted fraction change.

The mass mixing ratio is expressed as follows:

$$r_{mix} = \frac{m_{Mg(OH)_2}}{m_{hed}} \tag{6}$$

The mole reacted fraction change is showed in the equation 7:

$$\Delta_{x} = x - x_{ini} \tag{7}$$

x is the reacted fraction and

$$x = 1 + \frac{\Delta m / M_{H_2O}}{m_{M_g(OH)_2} / M_{M_g(OH)_2}}$$
(8)

Where Δm is the mass of water vapour moving out of the reactor. $m_{Mg(OH)_2}$ is the initial mass of Mg(OH)₂ in the reactor. M_{H_2O} is the molecule weight of the water (18.01 g/mol).

The related physical properties of EM8 block are shown in the table 2 [4].

Properties	Unit	Value
Mass mixing ratio (r _{mix})		8:9
Density of bed	g/cm ³	1.002
Heat storage capacity in one hours	MJ/m ³	700

Table 2. Physical properties of the EM8 block.

Choosing reactor material

The maximum service temperature of the material chosen to fabricate the reactor, steel grade $153MA^{TM}$ must be greater than the temperature of exhaust gas at the outlet of the engine (the maximum exhaust gas temperature was 1065 K in the current study or 1113 K in Tianyou experiments [5]). The properties of the steel grade $153MA^{TM}$ are shown in table 3 [6].

Properties	Unit	Value
Maximum service temperature	Κ	1273
Mass density	g/cm ³	7.8
Thermal conductivity	W/m.K	25.5
Heat capacity	J/kg.K	500

Table 3. 153MATM steel properties.

Reactor design

The reactor consists of two tubes: inner and outer tubes. EM8 block is stored inside the inner tube, and the exhaust gas flows in the space between the two tubes.



Figure 5. The reactor design.

Heat is transferred from the exhaust gas to EM8 block, and the dehydration reaction takes place inside the inner tube. Water vapour from the dehydration of $Mg(OH)_2$ flows out of the reactor from the vapour outlet placed at the top of the reactor. In the space between the two tubes, two wings are designed to make the temperature inside the reactor become even and to increase the moving time of the exhaust gas flow in the reactor. Figure 5 shows the initial design of the reactor with the design parameters listed in table 4.

Parameter	Unit	Value	
Inner tube			
Diameter	mm	100	
Thickness	mm	3.05	
Outer tube			
Diameter	mm	160	
Thickness	mm	3.05	
Exhaust gas inlet			
Diameter	mm	88.9	
Thickness	mm	3.05	
Exhaust gas outlet			
Diameter	mm	88.9	
Thickness	mm	3.05	
Vapour outlet			
Diameter	mm	88.9	
Thickness	mm	3.05	
Wings			
External diameter	mm	160	
Internal diameter	mm	53.05	
Thickness	mm	3.05	

Table 4. The design parameters of the reactor.

The parameters of exhaust gas at the exhaust gas inlet

It was proposed to install the reactor between the engine exhaust port and the catalytic converter. The temperature at the inlet of the reactor is assumed to be equal to the temperature at the engine exhaust port. This temperature and the volume percentages of exhaust gas components are given in table 5.

Parameter	Unit	Value
Temperature	Κ	1028
CO	%vol	0.1
CO ₂	%vol	15.5
HC	ppm	9.9
NO _x	ppm	2335.7
O ₂	%vol	0.2

Table 5. Information of the exhaust gas at the inlet of the reactor.

CFD simulation of the designed reactor

ANSYS Fluent was used to simulate the gas flows and heat transfer processes in the reactor. The input data are the initial design parameters, exhaust gas parameters and reactor material's thermochemical properties.

As the temperature of the exhaust gas at the engine exhaust port is high (1028K), the mixed thermal condition (combination of convection and radiation) model was chose to simulate the heat transfer between the exhaust gas and the reactor walls.

EM8 block is assumed as a solid material so the heat transfer process inside the EM8 block is assumed as the heat conduction process with the properties given in table 4.

It is assumed that the heat absorption process of EM8 block does not vary with time in one hours working time. The heat storage capacity in 1 hour is 700 MJ/m³.Equivalently the heat generator rate is 194.4 kW/m³.

Figure 6 illustrates the temperature contours of the exhaust gas inside the reactor.



Figure 6. The temperature distribution of the exhaust gas inside the reactor.

Simulation results in Figure 6 shows that the average temperature of exhaust gas over the cross section of exhaust gas outlet port is approximately 985K. This temperature was used to calculate the heat energy of exhaust gas at the outlet, and the amount of heat stored in the reactor. Results are shown in table 6.

Parameter		Value
Heat energy at the inlet of the reactor	kW	61.91
Temperature at the outlet of the reactor	Κ	985
Heat energy at the outlet of the reactor	kW	58.27
Energy stored in the reactor	kW	3.64
Percentage of energy stored	%	5.8
Volume of EM8 block stored in the reactor	dm ³	2.51
Mass of EM8 block stored in the reactor	kg	2.51

Table 6. Results of simulation for the process in the reactor.

As shown in table 6, with a small reactor and in one hour operating time, the chemical heat storage device can store 5.8% heat loss in the exhaust gas. The amount of stored heat depends on the size of the reactor, the temperature of exhaust gas at the exhaust gas inlet and the vehicle operating time.

EM8 block is stored in the reactor in the block state with the outer surface of EM8 block fits with the inner face of the inner tube of the reactor so the volume and mass of EM8 block can be calculated through reactor parameters. As shown in table 6, to store 5.8% of exhaust gas heat, the amount of EM8 block required is 2.51 kg. This mass is enough to use in one hour. After this period, almost $Mg(OH)_2$ in EM8 block is converted to MgO and heat is stored in the reactor.

Conclusions

To investigate the feasibility of chemical heat storage for saving the exhaust gas energy in an IC engine, experiments were conducted on a 6-cylinder spark ignition engine. The average percentage of heat lost is calculated based on the measurement data obtained from operating parameters of the engine such as engine torque, speed or components and the temperature of exhaust gas at the engine exhaust port. The study estimated the potential of chemical heat storage technology when incorporated with the engine to store a part of energy loss. The initial design was verified by numerically simulating the heat exchange processes inside the reactor in one hour working time. With 5.8% heat energy of exhaust gas stored in 2.51 kg of EM8 block, the chemical heat storage technology is feasible, and it is expected to be applicable as a heat storage system for vehicles.

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