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Numerical investigation of heat storage in a chemical heat storage system for saving exhaust gas energy in internal combustion engines

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Abstract. Thermal energy storage has become more and more important to improving the overall efficiency of energy systems by utilising the wasted energy. This study was aimed to develop a chemical heat storage (CHS) system using EM8block and its dehydration and hydration reactions to recover the thermal energy wasted by the exhaust gases in internal combustion (IC) engines. To experimentally investigate the performance of the CHS system in the heat storage process, a CHS system was developed and tested on a Diesel engine (D1146TI). To further investigate the CHS system in engine conditions more than that in experiments, a CFD model of the CHS system was developed using the commercial code of ANSYS FLUENT as a platform. In the 60 minutes mode, the maximum stored energy in the CHS system was 21.9 MJ which was equivalent to 4.78% of exhaust gas energy with 72.54% of the EM8block reacted at the full engine load. The stored energy and the percentage of reacted EM8block decreased with the decrease of the engine load. In the full charge mode, the simulation results showed that the time on fully charge of the CHS reduced with the increase of the engine load and that the shortest time was 67.1 minutes at full engine load. This time on full charging increased to 110.3 minutes at 50% engine load. The simulation results also showed that the maximum percentage of the exhaust gas energy stored in the CHS system was 7.14% at 70% engine load.

1. Introduction

Utilizing the wasted energy is one of the important strategies for addressing the current issue of sustainability by increasing the overall efficiency of the engine. Internal combustion (IC) engines have been widely used in many fields, such as transportation, construction or agricultural sectors. However, a significant amount of fuel energy has to be lost as wasted heat through exhaust gas. Some solutions to cover exhaust gas energy have been adopted including the thermoelectric generation (TEG) [1, 2], exhaust gas recirculation system (EGR) [3] and heat exchangers [4, 5]. However, the solutions convert and use the heat energy of exhaust gas instantaneously and may not be applicable in the situations which require to keep the stored energy until it is needed. Different from the instantaneous energy conversion systems, thermal energy storage (TES) that are applying in many fields, especially in concentrating solar power plant or in the building can store the energy until it is used.

Sensible, latent and chemical heat storages (CHS) are classified as TES. Sensible heat storage systems store heat energy based on the temperature changing of solid or liquid material. In the latent heat storages systems, the heat energy is stored in the latent heat of a phase change material. Different
from the physical TES systems above, CHS systems store and release heat energy through the reversible reaction of chemical material [6]. As the chemical products of CHS system are stored separately at the ambient temperature, the stored energy can be retained for a long time with small heat loss [7]. However, the structure of a CHS system is more complex than that of a physical heat storage system, resulting in higher initial cost [8].

CHS systems have been applied to storing the solar energy for domestic hot water, air-conditioning [6], and heat energy in the thermal power plant [9]. However, applying CHS to IC engines is still new. The research of Kabushiki Kaisha Toyota Jidoshokki [10] was the first one to propose the application of CHS to recovering exhaust gas energy to heat the catalyst in IC engines.

In the present study, a new CHS system consisting of a reactor with Mg(OH)\(_2\) as the initial chemical material has been developed and investigated to recover the exhaust gas energy of a diesel engine. The experiments were conducted to estimate the performance of the CHS system in the heat storage process at various engine operating conditions. In the heat output process, the stored energy was used to heat the engine intake air, aiming to extend this application to other heating required in IC engines and hybrid vehicles.

2. The principle of CHS using to recover exhaust gas energy of IC engine

The chemical material adopted in this research is Magnesium hydroxide (Mg(OH)\(_2\)) based on its reversible reaction. To store the heat energy of the exhaust gas, it was proposed that two main devices would be installed in the exhaust gas pathway of an IC engine, a reactor and a water tank. The reactor is located between the engine exhaust port and the catalytic converter. The principle of the heat storage process is shown in Figure 1.

![Figure 1: The heat storage process](image)

In the heat storage process, heat is transferred from the exhaust gas to Mg(OH)\(_2\) and converts to magnesium oxide (MgO) and water vapour (H\(_2\)O) in the dehydration reaction in the reactor. During this process, MgO is retained inside the reactor, the water vapour moves into and condenses in the water tank.

However, the thermal conductivity of the pure Mg(OH)\(_2\) is very low (within 0.15-0.16 W/m.K [9]). To increase the heat transfer efficiency, a new compound was proposed by Massimiliano [9]. It was the combination of Mg(OH)\(_2\) and expanded graphite (EG) with the mass ratio of 8:1 and in the block state (EM8block). EM8block was adopted in the present study. As reported in [9], the advantages of this material compared with pure Mg(OH)\(_2\) include: high thermal conductivity, great density, reduced void fraction of the bed. The main properties of Mg(OH)\(_2\) pellets and EM8block are shown in Table 1.

| Parameter              | Unit | Mg(OH)\(_2\) pellets | EM8block |
|------------------------|------|-----------------------|----------|
| Density of bed         | g/cm\(^3\) | 0.966                 | 1.002    |
| Working temperature    | °C   | 250-800               | 250-800  |
| Reaction enthalpy      | kJ/mol | 81                    | 81       |
| Thermal conductivity   | W/m.K | 0.15-0.16             | 1.5-1.7  |
3. apparatus and methods

Experiments were conducted on the D1146TI diesel engine in the Engine Laboratory at the Hanoi University of Science & Technology in Vietnam. D1146TI is a 4-stroke 6-cylinder Diesel engine for trucks in Vietnam. Figure 2 shows a photo of the experiment apparatus set up in the AVL engine test-bed and the schematic diagram of the test rig.

Three thermostats were placed to measure the exhaust gas temperatures at the inlet and outlet of the reactor (T₁, T₂), EM8block temperature (T₃) in the heat storage process and the engine intake air temperatures at the reactor inlet and outlet (T₄, T₅), the wall temperature of the tube of the reactor (T₆) in the heat output process. Each experiment was performed in four stages.

- **Stage 1 (The heating stage):** the temperature of EM8block (T₃) increased from the ambient temperature to around 80-90°C.
- **Stage 2 (The heating and evaporating stage):** the moisture inside EM8block evaporated and moved to the water tank until T₃ was around 110-120°C.
- **Stage 3 (The heating stage):** EM8block was heated to the reaction temperature of Mg(OH)₂ (T₃ was around 250-280°C).
- **Stage 4 (The heating and storing stage):** The CHS system was heated continuously and the dehydration reaction of EM8block occurred in the reactor.

To investigate the CHS system in engine conditions more than that in experiments, a CFD model of the CHS system was developed using the commercial code of ANSYS FLUENT as a platform. The model was verified by comparing the simulation results with the experimental ones. The verified model was then used to test the CHS system, which was further improved from the one used in the experiments.

4. Performance of CHS in the heat storage process

In the heat storage process, the performance of the CHS system in the current study was investigated in two time modes including 60 minutes mode and the full charge mode.

In 60 minutes mode, the engine run in 60 minutes and the criteria for evaluating the performance of CHS includes.
- The percentage of the stored exhaust gas energy.
- The percentage of the reacted EM8block.

In the full charge mode, the engine run until all EM8block inside the reactor reacted. In this mode the performance of CHS is presented by criteria as follows:
- The percentage of the stored exhaust gas energy.
- The full charge time.

4.1. 60 minutes mode

It can be seen from Figure 3 that the percentage of reacted EM8block in 60 minutes mode highly depends on the engine load. At 50% engine load, 60 minutes after the engine started, only 9.6% EM8block reacted inside the reactor. It increased 7.55 times to 72.54% at the full engine load. At the engine load lower than 50%, the low exhaust gas temperature led to the low performance of the CHS system and applying the CHS system in this case is ineffective. As shown in Figure 4, the stored energy increased with the increase of the engine load from 2.9 MJ at 50% engine load to 21.9 MJ at the full engine load. The percentage of the exhaust gas energy stored in the CHS system was highest at 70%, 80%, 90% engine loads with around 5.05%. This percentage decreased sharply when the engine load was smaller than 70% to 3.69% at 60% engine load and 1.26% at 50% engine load. The reason was the low temperature of the exhaust gas at the low loads of the engine led to the longer heating time (stages 1, 2 and 3), so the storing time (stage 4) was shorter and the stored energy was smaller. Besides, at the full engine load, the percentage of the stored exhaust gas energy was slightly decreased at 4.78%. The reason was the increase rate of the exhaust gas energy was higher than the stored energy.
After 60 minutes, when the engine kept running, the dehydration reaction of EM8block continuously occurs inside the reactor until all EM8block reacted. As shown in Figure 5, the longest full charge time was at 50% engine load at 110.3 minutes. This time decreased 67.1 minutes at the full engine load. It can be seen that at the higher engine load, the temperature of the exhaust gas was higher and the heating effect of the exhaust gas was stronger. It contributed to the shorter charge time of the CHS system.

As shown in Figure 6, the percentage of the stored exhaust gas energy changed slightly when the engine load changed from 50% to full engine load. The highest percentage of the stored exhaust gas energy was 7.14% at 70% of engine load, and it reduced when the engine load increased or decreased. At the higher engine loads, the full charge time decreased; however, the energy of the exhaust gas energy per unit time increased. On the contrary, at the lower engine loads, the energy of the exhaust gas per unit time decreased, but the full charge time was longer. All of them led to the total energy of the exhaust gas increased and the percentage of the stored exhaust gas energy in the whole charge time decreased compared with that at 70% engine load.

Table 2: Main properties of CHS system in the current study and other TES systems to recover exhaust gas energy of IC engines

| Parameter                           | Pandiyarajan TES system [11]       | Pertti TES system [12]               | M.Gumus TES system [13]       | Tessa TES system [14]         | CHS system in the current study |
|-------------------------------------|------------------------------------|-------------------------------------|--------------------------------|--------------------------------|--------------------------------|
| Applications                        | Heating the engine oil             | Heating the engine                  | Heating the engine            | Heating the engine, the cabin | Heating the intake air          |
| Size                                | A heat exchanger: 450 mm ID x 720 mm H | A accumulator: 195 mm OD x 300 mm H | A stored tank: 220 mm OD x 400 mm L | A stored tank: 610 W x 710 D x 230 H mm | A reactor: 360 mm OD x 500 mm H |
|                                     | A TES tank: 323 mm ID x 500 mm H   | Two plate heat exchangers: 190 mm x 170 mm | A water tank: 20 mm OD x 30 mm H |                                |                                |
| Stored energy                       | 19,500 kJ                          | 2500 kJ                             | 2277 kJ                       |                                | 30,197 kJ                      |
| Percentage of stored exhaust gas energy | 11% at 50% engine load 14% at 75% engine load 15% at full engine load |                                 |                                |                                | 6.5% at 50% engine load 7.14% at 70% engine load 6.1% at full engine load |
| Full charge time                    | 180 min at 50% engine load         |                                     |                                |                                | 110 min at 50% engine load     |
Compare with other TES systems applying to recover exhaust gas energy of IC engine vehicles, the CHS in the current study has a higher stored energy and the longer storing time as shown in table 2.

5. Conclusion
To investigate the performance of the CHS using Mg(OH)$_2$, experiments were conducted at 60%, 70% and 80% engine loads in 60 minutes. Numerical simulations were performed using the commercial CFD code ANSYS FLUENT as the platform and verified by comparing the simulation and experimental results. The verified model was used to investigate the performance of the CHS system at condition different from that in experiments.

In 60 minutes mode of the heat storage process, the maximum percentage of the reacted EM8 block was 72.5% at the full engine load. This number decreased to 9.6% at 50% engine load. The highest percentage of the stored exhaust gas energy was 5.05% at 80% engine load and it dropped to 1.26% at 50% engine load.

In the full charge mode, the full charge time of the CHS system depended on the engine load, and the shortest time was 67.1 minutes at the full engine load. This time increased with the decrease of the engine load and it took 110.3 minutes at 50% of engine load. The variation of the percentage of stored exhaust gas energy with the engine load was insignificant. The highest percentage was 7.14% at 70% engine load, and it decreased slightly when the engine load changed. The smallest percentage of the stored exhaust gas energy was 6.27% at the full engine load.

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