CHEMICAL HEAT STORAGE FOR SAVING EXHAUST GAS ENERGY IN INTERNAL COMBUSTION ENGINES

By

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A thesis in fulfilment of the requirement for the degree of

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Under the supervision of Associate Professor **Guang Hong**

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Certificate of Original Authorship

I, Duc Luong Cao declare that this thesis is submitted in fulfilment of the requirements for the award of Doctoral degree in the School of Mechanical and Mechatronic Engineering, Faculty of Engineering and Information Technology, at the University of Technology Sydney.

This thesis is wholly my own work unless otherwise reference or acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

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List of Publications

Journal Articles

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Conference proceedings

[1] **Duc Luong Cao**, Guang Hong, Jack Wang. Preliminary investigation to the feasibility of chemical heat storage for saving the exhaust gas energy in a spark ignition engine. *The 20th Australasian Fluid Mechanics Conference*, Australasian Fluid Mechanics Society, Perth Australia 2016.

[2] **Duc Luong Cao**, Guang Hong, Tuan Anh Le. Preliminary comparison of chemical heat storage systems for saving exhaust gas energy in gasoline and diesel engines.*11th Asia-Pacific Conference on Combustion,* The combustion Institute, Sydney Australia 2017.

[3] **Duc Luong Cao**, Guang Hong, Tuan Anh Le. Investigation of chemical heat storage processes for recovering exhaust gas energy in internal combustion engines. T*he 21st Australasian Fluid Mechanics Conference*, Australasian Fluid Mechanics Society, Adelaide Australia 2018.

[4] **Duc Luong Cao**, Guang Hong, Tuan Anh Le. Numerical investigation of heat storage in a chemical heat storage system for saving exhaust gas energy in internal

combustion engines. *Internal conference on Sustainable Energy and Green Technology*. Bangkok, Thailand 2019

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Nomenclatures

Symbol	Description	Unit
A	Area	m^2
C_{ex}	Specific heat of the exhaust gas	kJ/kg.K
$C_{EM8block}$	Specific heat of EM8block	kJ/kg.K
C_r	Specific heat of the reactor	kJ/kg.K
$E_{captured}$	Captured energy of the reactor	kW
E_{com}	Energy of exhaust gas components	kW
E_{ex}	Energy of the exhaust gas	kW
$E_{EM8lock}$	Energy for heating EM8block	kW
E_{other}	Other energy losses and storage	kW
E_r	Energy for heating the reactor	kW
E_{total}	Total energy of IC engine	kW
h	Heat transfer coefficient	$W/m^2.K$
h_{com}	Enthalpy of the exhaust gas component	kJ/kg
k_d	Dehydration rate of EM8block	s^{-1}
m_a	Intake air mass flow rate	kg/s
m_{air}	Air mass flow rate	kg/s
m_{com}	Exhaust gas component mass flow rate	kg/s
m_{ex}	Exhaust gas mass flow rate	kg/s
$m_{EM8block}$	Mass of reacted EM8block	kg

m_{fuel}	Fuel mass flow rate	kg/s
m_{H_2O}	Mass of water vapour generating in the dehydration reaction	kg
	Mass of condensed water in the water tank in the heat storage process	
$m_{Mg(OH)_2}$	Mass of $Mg(OH)_2$ in EM8block	kg
m_r	Mass of the reactor	kg
m_{total}	Total mass of EM8block	g
M_{H_2O}	Mole mass of the water	g/mol
$M_{Mg(OH)_2}$	Mole mass of $Mg(OH)_2$	g/mol
$q_{d,v}$	Volumetric storage capacity of the dehydration reaction	kJ/m^3
$q_{h,v}$	Volumetric storage capacity of the hydration reaction	kJ/m^3
$Q_{ex,in}$	Total energy of the exhaust gas at the reactor inlet	kJ
$Q_{ex,out}$	Total energy of the exhaust gas at the reactor outlet	kJ
Q_{HV}	Heating value of the fuel	kJ/kg
Q_{stored}	Stored energy inside the reactor in the heat storage process	kJ
$r_{captured}$	Percentage of the captured exhaust gas energy of the reactor	%
r_{com}	Mass percentage of the exhaust gas component	%
$r_{EM8block}$	Percentage of the reacted EM8block	%
r_{mix}	Mass mixing ration.	
r_{stored}	Percentage of stored exhaust gas energy	%
S	Heat source inside EM8block	kJ/m^3

t	Time	s
T_1	Exhaust gas temperature at the reactor inlet in the heat storage process	^0C
T_2	Exhaust gas temperature at the reactor outlet in the heat storage process	^0C
T_3	Temperature of EM8block in the heat storage process	^0C
T_4	Intake air temperature at the reactor inlet in the heat output process	^0C
T_5	Heated air temperature at the reactor outlet in the heat output process	^0C
T_6	Temperature of the reactor wall in the heat output process	^0C
T_a	Average temperature of the intake air in the reactor	^0C
T_w	Temperature of the reactor wall	^0C
T_{ex}	Temperature of the exhaust gas	^0C
x_d	Reacted fraction of the dehydration reaction	
x_d^0	Initial reacted fraction of the dehydration reaction	
$V_{Em8block}$	Volume of EM8block inside the reactor	m^3
Δx_d	Mole reacted fraction change of the dehydration reaction	
Δx_h	Mole reacted fraction change of the hydration process.	
$\Delta\tau$	Time step	s
ΔH_r^o	Reaction enthalpy of the dehydration reaction	kJ/mol
$\rho_{EM8block}$	Density of EM8block	kg/m^3
α_{ex}	Convection heat transfer coefficient of the exhaust gas	$W/m^2.K$

λ_{ex}	Thermal conductivity of the exhaust gas	W/m.K
λ_r	Effective thermal conductivity of the reactor wall	W/m.K
ϵ	Emission coefficient of the wall	
σ	Stefan - Boltzman constant	

Abbreviations

ASC	Ammonia Slip Catalyst
CFD	Computational fluid dynamics
CHS	Chemical heat storage
DHW	Domestic hot water
DNS	Direct Numerical Simulation
DOC	Diesel Oxidation Catalyst
DPF	Diesel Particulate Filter
EG	Expanded graphite
EGHR	Exhaust gas heat recovery
EM4	Compound of $Mg(OH)_2$ and EG in the mass mixing ratio of 4:1
EGR	Exhaust gas recirculation system
EM8	Compound of $Mg(OH)_2$ and EG in the mass mixing ratio of 8:1
EM16	Compound of $Mg(OH)_2$ and EG in the mass mixing ratio of 16:1
EM8block	Compound of $Mg(OH)_2$ and EG in the mass mixing ratio of 8:1 in block state
$EM8block_p$	Solid product of the dehydration reaction of EM8block
HVAC	Heating, ventilation and air conditioning
LES	Large Eddy Simulation
NEDC	New European Driving Cycle
PCM	Phase change material

RANS	Reynolds Averaged Navier-Stokes Simulation
SCR	Selective Catalytic Reduction
SST	Shear Stress Transport
TEG	Thermoelectric generation
TES	Thermal energy storage

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Abstract

Utilizing the wasted energy is one of the important strategies for addressing the current issue of sustainability by increasing the energy system overall efficiency. Thermal energy storage (TES) systems have been in development to address the above strategy by storing the wasted energy and reusing it when needed. Chemical heat storage (CHS) system is one kind of TES systems, with its advantages of high energy density and long storage time and has been studied in recent years. CHS systems have been applied to storing the solar energy for domestic hot water, air-conditioning, etc. and heat energy required in the thermal power plants. However, research is needed to exploit more applications of CHS to store and utilize the wasted heat energy.

Internal combustion (IC) engines have been and are still the main power resource for vehicles and stationary electricity generation systems. However, the heat lost through the exhaust gases of an IC engine is significant and it is the major factor limiting the engine thermal efficiency. Technologies for instantaneously converting the heat energy of the engine exhaust gas to be other forms of energy have become mature, such as thermoelectric generation (TEG) and heat exchangers. Difference from them, CHS stores the wasted energy and reuses it when needed. However, applying CHS in the IC engine is still new. This study was aimed to develop a CHS system using magnesium hydroxide ($Mg(OH)_2$) and its dehydration and hydration reactions to store the engine exhaust gas energy rather than instantaneous energy conversion until the stored energy was need.

To experimentally investigate the performance of the CHS system, a CHS system was developed and tested on a Diesel engine (D1146TI). In the heat storage process, the experiments were conducted at 60%, 70% and 80% engine load conditions. Experimental

results showed that at 80% engine load, 61.4% of chemical material reacted and 5.05 % heat energy of exhaust gas was stored in an hour. The percentage of the stored exhaust gas energy reduced with the decrease of engine load due to the decrease of the exhaust gas energy. In the heat output process, as one of the proposed applications, the engine intake air was heated with the stored energy by hydrating MgO at the ambient temperature. The experimental results showed that the intake air could be heated to the temperature 5.7^0C - 17.3^0C higher than the ambient temperature of 23^0C.

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. The model was verified by comparing the simulation and experimental results. In the heat storage process and 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. In the heat output process, the CFD model was used to test the CHS system at different ambient temperature values. Simulation results showed that the temperature of the engine intake air heated by the CHS could be increased from the ambient temperature of -10^0C to 12.15^0C.

Numerical simulation was also performed to investigate the CHS system modified with two wings added to the exterior wall of the tube of the reactor, aiming to enhance the heat transfer between the exhaust gas and the reactant. In the heat storage process in 60 minutes mode, both the percentage of the stored exhaust gas energy and reacted EM8block increased. Compared with the original CHS system, the percentage of reacted EM8block increased from 72.54% to 81.6% and the percentage of stored exhaust gas energy increased from 4.78% to 5.47% at the full engine load. The effect of the modified CHS system became stronger with the increase of the engine load. In the full charge mode, using the modified CHS system, the full charge time reduced 3.1 minutes at the full engine load and 8.2 minutes at 50% engine load compared with the original CHS system. Furthermore, the maximum percentage of stored exhaust gas energy increased from 7.14 % to 7.58% at 70% engine load. In the heat output process, the effect of the modified CHS system was stronger at the lower ambient temperature and higher reactor wall temperature. In the same condition at the ambient temperature of -10^0C and the reactor wall of 85^0C, the heated air temperature in the modified CHS system was 1.2^0C higher than that in the original one.