Numerical study of using different Organic Rankine cycle working fluids for engine coolant energy recovery

Fenfang Chen\textsuperscript{a}, Yiji Lu\textsuperscript{b*}, Xiaoqiang Chen\textsuperscript{a}, Zhi Li\textsuperscript{a}, Xiaoli Yu\textsuperscript{a}, Anthony Paul Roskilly\textsuperscript{b}

\textsuperscript{a} Department of Energy Engineering, Zhejiang University, Hangzhou, 310027, China
\textsuperscript{b} Sir Joseph Swan Centre for Energy Research, Newcastle University, Newcastle, NE1 7RU, UK

Abstract

Engine waste heat recovery technology especially Organic Rankine cycle (ORC) has been widely studied in order to achieve higher overall thermal efficiency, reduce the engine emissions and improve the fuel economy. The coolant energy occupies around 30\% of the fuel energy can be used as the heat source for ORC system. This paper studies thermal status of the engine heated components when using different ORC working fluids as engine coolant to avoid the heat loss using heat exchanger to transfer coolant to the ORC fluid. A Solid-Liquid Conjugated Heat Transfer (SLCHT) calculation method is developed to calculate the heat transfer inside the engine, which can solve the temperature field of both solid zone and fluid zone. The simulation results have been validated by the experimental data from a 6-cylinder medium duty diesel engine, when water is the coolant in the system. The simulation model is then used to predict the temperature profile using different ORC working fluids and investigate the influence of different ORC working fluids on the cooling effects of the engine heated parts. The maximum temperature of the heated components has been selected as the evaluation parameters. The results reveals that applying selected ORC working fluids in engine as coolant is not practical under the designed conditions, which will make the engine overheated. Further investigation showed that increasing mass flow rate of the coolant can decrease the thermal status of the heated components but still cannot meet the cooling demands even under 200\% of the original mass flow rate. The variations of the coolant outlet temperature and exergy were also analysed.

© 2017 The Authors. Published by Elsevier Ltd.
Peer-review under responsibility of the scientific committee of the 9th International Conference on Applied Energy.

Keywords: Organic Rankine cycle, Coolant energy recovery, Solid-Liquid Conjugated Heat Transfer, Internal Combustion Engine
1. Introduction

Engine waste heat recovery technologies especially Organic Rankine cycle (ORC), which is one of the most practical methods to recover waste heat of Internal Combustion Engine (ICE), attract ever increasing attentions due to the environmental problems and requirement on the development of high efficiency energy system [1-3]. The engine coolant and exhaust energy respectively occupies 30% and 40% of the overall fuel energy, which are two main heat sources to drive the engine waste heat recovery system [4, 5]. Majority researches conducted for the engine waste heat recovery are mainly focusing on the utilisation of exhaust gas due to its relatively higher temperature profile, which can potentially be used to drive more efficient heat driven system compared with that of coolant energy recovery system [6-8]. However, the effectively recovery of coolant energy with a well-designed system layout can potentially and effectively improve the overall energy efficiency of the ICE and reduce the engine emissions [9, 10]. The current research barrier to use the coolant energy from the ICE is because of the low temperature profile form the engine coolant, which is commonly between 80-95 °C [11]. In other words, the exergy of coolant water is quite low, making it very difficult to be recovered when heat exchanger is used to transfer the heat energy from the coolant to the ORC working fluid. The potential solution to avoid the heat transfer losses is to use the ORC fluid as the coolant to directly cool down the engine and recover the coolant energy [12, 13].

In order to study the potential of using ORC working fluid as engine coolant, the thermal status of the engine heated components is critical to be evaluated, which will affect the engine performance, emissions and durability. Mover, the operation parameters of the temperature increase of the ORC working fluid after flowing through the engine water jacket should be confirmed. In this paper, a Solid-Liquid Conjugated Heat Transfer (SLCHT) simulation model has been used to calculate the complicated flow and heat transfer process in ICE. With this method, temperature fields of both engine heated components and coolant fluid with different fluids being used as engine coolants can be solved. The temperature field is used to evaluate the thermal status of heated components.

2. Description of the simulation model

2.1. Calculation Principle

The heat transfer within the solid zone and the liquid zone is described by the steady heat conduction equation. And for the solid-liquid interface, the Fourier heat equation and the convective heat transfer control equation are established.

The coolant in the water jacket can be considered as viscous, incompressible turbulent flow in 3D numerical calculation. Besides the continuity equation, momentum equation and energy equation, turbulence model are used in
this study as well. For the consideration of both computing time and accuracy, the standard k-ε turbulence model is chosen. However, the standard k-ε turbulence model only applicable to the fully developed turbulence, and the standard wall function is employed to simulate the influence of the wall on the turbulence in near-wall region. The equations described above can be found in the previous published paper by the authors [14] and are solved in computational fluid dynamic software STAR-CCM+.

2.2. Discretization of the model

The model includes the solid zone of cylinder head, liner, engine block and the liquid zone of coolant fluid, and is modelled in 3D modelling software. In order to bring convenience for establishing the meshing model and decrease the grid number, appropriate simplification was made while modelling. Small features like small bolts and chamfer angles that have little effect on simulation results but will greatly increase the mesh number were removed. Then the mesh was created in 3D CFD software STAR-CCM+ automatically, shown as Fig.1 and Fig.2.

2.3. Boundary Conditions

Boundary condition is the key factor in simulation and directly affects the calculation accuracy. In the engine, the main boundary condition is the combustion chamber that directly contact with high temperature combustion gas. The flow and chemical reaction in combustion chamber is rather complicated and cannot be accurately solved. So, in this paper, average temperature and average Heat Transfer Coefficient (HTC) were adopted for the convection heat transfer between the gas and solid wall. The one-dimensional thermal dynamic model was developed in engine work process simulation software AVL Boost, by which space average temperature and HTC can be solved. Then time average temperature and HTC in a working cycle can be calculated with following equations:

Because the timing and the duration of touching the combustion gas on each position of the inner surface of the liner are not same in one cycle, and the gas temperature and flow velocity in each location near the cylinder head fire face are also different, distribution functions of temperature and HTC in the inner surface of the block were adopted to describe these spatial variations of heat transfer.

The specification of the boundary condition determination of each surface can also be found in literature [12].
3. Validation of the simulation model

Engine test was taken to verify the accuracy of the simulation. Thermocouples were used for the measurement of the cylinder head temperature field. The arrangement of the measuring points on cylinder head is shown in Fig.3. Then the cylinder head was assembled in the engine for test. The engine was firstly started for break-in for about 30 minutes. Then it was set to the 1900 r/min and 100% load (rated operation), keep running until it reach thermal equilibrium. The temperature data measured by thermocouples were collected by data acquisition equipment of NI Corporation and were plotted in Fig.4.

It is can be seen from the figure that the difference between the calculated values and the experimental values on the points in the cylinder block is small, generally less than 5%. The maximum difference is 5.45% at measure point 12. It indicates that the boundary conditions applied on the model is appropriate and the method established in this paper is practical, which can be used in further investigations.

4. Results and discussion

![Fig.5. temperature field of the 5th cylinder head fire face with different working fluids](image)

The numerical studies were carried out with different working fluids of R113, R123, R141b, R245ca, R245fa and isopentane, which have been widely used for ORC system [15, 16]. The mass flow rate was kept at 6.67 kg/s and the pressure was considered at 3.0MPa to avoid boiling and evaporation in the water jacket. Fig.5 shows the temperature fields of the 5th cylinder head fire face, from which we can see that the thermal state of the engine is greatly affected by the working fluids. The maximum temperature of cylinder head and liner are generally high with selected fluids as shown in Fig.6. The maximum temperature of cylinder head and liner is 390.77 ℃ and 411.72 ℃, respectively when use R113 as coolant. Note that the maximum temperature that liner and cylinder head (Grey Iron) can endure is 380 ℃. And for liner, the temperature near the first piston ring when the piston is at top dead centre should be lower than 220 ℃, otherwise the lubrication oil will be deteriorated under high temperature. Furthermore, even if the maximum temperature has not reach the critical temperature of the heated components, high cylinder wall temperature will cause deterioration of the in-cylinder combustion, leading to low thermal efficiency and bad emission of the engine. It can be concluded that using selected working fluids under the designed working conditions as engine coolant may cause the performance degradation or even the failure of the heat components under original mass flow rate.

Coolant outlet temperature is an important operational condition, which plays critical role in both engine thermal balance and the energy flow in engine heat recovery system. The coolant outlet temperature and energy when use different working fluids are plotted in Fig.7 and obvious variations in these two parameters can be observed. Results show that coolant outlet temperature is highest when use R113 as coolant, which is 95.48 ℃, while that of water is the lowest. But trend of coolant outlet energy is just on the contrary. It can be explained by that the specific heat of R113, R123, R141b, R245ca, R245fa, isopentane and water goes up respectively. The temperature of the coolant
with low specific heat increases more when absorbing certain amount of heat, and the temperature difference between coolant and heat components will be smaller, leading to lower heat exchange rate in convection heat transfer. It also indicates that specific heat is one of the most critical physical parameters when choosing coolant fluids.

Fig.6. Maximum temperature of the liner and cylinder head with different working fluids

Fig.7. Engine outlet temperature and coolant energy with different working fluids

Fig.8. Maximum temperature of the liner and cylinder head under different mass flow rate for each working fluids

Fig.9. Coolant outlet temperature and Exergy under different mass flow rate

From above analysis we can see that the thermal load of the heated components are extremely heavy while using selected working fluids. Lowering the thermal loads of the engine is of great significance. Then numerical study under various mass flow rate with these 6 working fluids were carried out. The mass flow rate of water was not changed for the purpose of comparison. Since the thermal load of the engine is high at original mass flow rate of 6.67 kg/s, the mass flow rate selected is 120%, 140%, 160%, 180% and 200% of the original data. Simulation results of maximum temperature of the cylinder head with selected working fluids under different mass flow rate is plotted in Fig.8, which indicate with the increase of mass flow rate, the temperature of the heated components decreases. This is because increasing mass flow rate can simultaneously raise the flow velocity of the coolant in water jacket and hence, strengthen the heat transfer in the interfaces of fluid and solid. Results show that a temperature decrease of 22.5-38.9 °C can be obtained when mass flow rate of coolant increased from original value.
to 200% of it. But the maximum temperature of the cylinder head under 200% mass flow rate is still higher than it under original value. It can be predicted that the thermal loads of the heated components can be reduced to original level if we increase mass flow rate continuously. Fig.9 shows the variations of coolant outlet temperature and exergy with the increase of coolant mass flow rate. It can be seen that coolant outlet exergy increases with the increase of mass flow rate, though coolant outlet temperature decreases.

However, higher mass flow rate will cause the increase of frictional resistance and then consume more pump power. Calculations shows that more than 10 times more friction power dissipation will be caused if mass flow rate increases by 100%.

5. Conclusions

- In this paper, a Solid-Liquid Conjugated Heat Transfer (SLCHT) calculation method to calculate heat transfer in multi-cylinder ICE was developed. The method was applied in a 6-cylinder medium duty diesel engine and the maximum error between simulation results and experiment dates is 7.56%. With this method, temperature fields of both heated components and coolant of multi-cylinder ICE can be solved precisely.
- With the same SLCHT method, calculations were done by using R113, R123, R141b, R245ca, R245fa and isopentane are ICE coolant and keeping mass flow rate at 6.67 kg/s. Results showed that the engine will be overheated with all selected working fluids under the same designed conditions as water.
- Specific heat is a critical physical parameters that determine the cooling effects. Coolant fluids with higher specific heat can take more heat away from the engine and have lower temperature increase, in other words, can achieve better cooling effects.
- When increase coolant mass flow rates to 120%, 140%, 160%, 180% and 200% of the original value, simulation results showed the thermal loads of engine heated components decreased with the increase of coolant mass flow rate but still cannot be reduced to original level when water is used to be coolant at the original mass flow rate of 6.67 kg/s. Simulations also showed coolant outlet exergy increases and coolant outlet temperature decreases with the increase of mass flow rate.

Acknowledgements

The authors would like to thank the support from NSFC-RS Joint Project under the grant number No. 5151101443 and IE/151256.

Biography

Dr Yiji Lu, born in June 1989, is currently a research associate in Newcastle University. He graduated from Shanghai Jiao Tong University in 2011 for his bachelor degree, he conducted his M.Phil. and Ph.D. in Newcastle University in 2012 and 2016. His Ph.D. program was fully sponsored by EPSRC and was awarded the '2015 Chinese Government Award for Outstanding Self-financed Students Abroad’ from China Scholarship Council. His research interests include but not limited to advanced waste heat recovery technologies, engine thermal management, advanced engine development, engine emission technologies, chemisorption cycles and expansion machines for power generation system. He has been regularly invited to review the manuscripts for the scientific journals including Applied Energy, Applied Thermal Engineering, Energy (the International Journal), and Energy for Sustainable Development.

References