МОДЕЛЮВАННЯ ТА ОПТИМІЗАЦІЯ В ТЕХНОЛОГІЇ КОНСТРУКЦІЙНИХ МАТЕРІАЛІВ

SIMULATION AND OPTIMIZATION IN TECHNOLOGY OF CONSTRUCTION MATERIALS

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MODELING OF SUPERCRITICAL CARBON DIOXIDE SYSTEMS IN DIESEL ENGINES IN THE OIL AND GAS INDUSTRY

МОДЕЛЮВАННЯ СИСТЕМ НАДКРИТИЧНОГО ДВООКИСУ ВУГЛЕЦЮ В ДИЗЕЛЬНИХ ДВИГУНАХ НАФТОГАЗОВОЇ ГАЛУЗІ

The article investigates the issue of modeling and increasing the fuel efficiency of power drives used on large-capacity diesel engines in the oil and gas industry. The use of supercritical carbon dioxide (sCO_2) cycles is proposed as a promising direction for the modernization of these diesel engines. An analysis of modern scientific research and publications on the topic of power drive modeling is carried out, and a number of unresolved problems related to the practical implementation of sCO_2 technology in the oil and gas industry are also identified. For this reason, the article considers the potential of using supercritical carbon dioxide (sCO_2), the organic Rankine cycle (ORC) and thermoelectric generator systems (TEG) for waste heat recovery (WHR) of technological transport in the oil and gas industry. The modeling results show that sCO_2 systems have the highest level of energy recovery from exhaust gases, surpassing ORC. In particular, the sCO_2 system was able to recover 19.5 kW in the maximum effective power mode and 10.1 kW in the maximum torque mode, while the ORC system — 14.7 kW and 7.9 kW, respectively. In the low effective power mode, the sCO_2 provided 4.2 kW, while the ORC — 3.3 kW. At the same time, the TEG system demonstrated significantly lower performance: 533 W at maximum effective braking power, 126 W at maximum torque and only 7 W in the low power and torque mode, which is explained by its lower efficiency compared to sCO_2 and ORC. Based on the results obtained, it was concluded that the sCO_2 and ORC technologies have the greatest potential for increasing the efficiency of WHR exhaust systems. The prospects of using supercritical carbon dioxide cycles to improve the economic characteristics of power drives in the oil and gas industry were separately noted.

***Keywords**: powertrain modelling; oil and gas transportation; diesel engine; waste heat recovery; supercritical carbon dioxide; organic Rankine cycle; thermoelectric generator; fuel efficiency.*

У статті досліджується питання моделювання та підвищення паливної ефективності силових приводів, що застосовуються на великокубатурних дизельних двигунах в нафтогазовій галузі. Як перспективний напрям модернізації зазначених дизельних двигунів запропоновано використання надкритичних циклів двоокису вуглецю (sCO_2). Проведено аналіз сучасних наукових досліджень і публікацій, присвячених тематиці моделювання силових приводів, а також виявлено ряд невирішених проблем, що стосуються практичного впровадження технології sCO_2 у нафтогазовій промисловості. З цієї причини у статті розглянуто потенціал застосування надкритичного двоокису вуглецю (sCO_2), органічного циклу Ренкіна (ORC) і термоелектричних генераторних систем (TEG) для рекуперації тепла відпрацьованих газів (WHR) технологічного транспорту нафтогазової галузі. Результати моделювання свідчать, що системи sCO_2 мають найвищий рівень енергетичного відновлення з вихлопних газів, перевершуючи ORC. Зокрема, система sCO_2 змогла відновити 19,5 кВт у режимі максимальної ефективної потужності та 10,1 кВт у режимі максимального крутного моменту, тоді як система ORC — 14,7 кВт і 7,9 кВт відповідно. У режимі низької ефективної потужності sCO_2 забезпечила 4,2 кВт, тоді як ORC — 3,3 кВт. При цьому система TEG продемонструвала значно нижчі показники: 533 Вт при максимальній ефективній потужності гальмування, 126 Вт при максимальному крутному моменті та лише 7 Вт у режимі низьких потужності й моменту, що пояснюється її меншою ефективністю порівняно з sCO_2 і ORC. На основі отриманих результатів зроблено висновок, що технології sCO_2 та ORC мають найбільший потенціал для підвищення ефективності вихлопних систем WHR. Окремо відзначено перспективність застосування надкритичних циклів двоокису вуглецю для покращення економічних характеристик силових приводів у нафтогазовій промисловості.

***Ключові слова**: моделювання силових приводів; нафтогазовий транспорт; дизельний двигун; утилізація відпрацьованого тепла; надкритичний вуглекислий газ; органічний цикл Ренкіна; термоелектричний генератор; паливна економічність.*

Problem's Formulation

For many decades, diesel engines have been widely used in oil and gas technological transport, drilling rigs, and various units within the oil and gas industry. One of the key challenges for professionals in this field is reducing fuel consumption and minimizing the toxicity of exhaust gases. It is important to note that 60—70 % of fuel energy is lost through the exhaust and cooling systems [1]. Waste heat recovery systems can partially compensate for these losses by converting a portion of the wasted heat into electricity. This energy can be used to reduce the load on the vehicle's generator, as well as to power fuel, oil, and water pumps, and other auxiliary engine drives, thereby contributing to fuel savings.

There are three promising systems currently being explored in the industry for use in internal combustion engine waste heat recovery systems [2]: thermoelectric generators (TEGs), Organic Rankine Cycle (ORC) systems, and supercritical carbon dioxide (sCO_2)-based systems [3]. These systems can be used not only for recovering heat from internal combustion engine exhaust gases but also in many other sectors, such as fossil-fuel-based power generation or marine energy systems [4]. These particular systems were selected because they are at the highest level of technological readiness compared to other emerging options (e.g., thermoacoustic systems), which are still in the early and mid-research stages [5].

Analysis of recent research and publications

Supercritical Carbon Dioxide (sCO_2) Cycles

Carbon dioxide is an environmentally friendly natural working fluid that is inexpensive, non-flammable, explosion-proof, and widely available in nature [6]. Additionally, carbon dioxide has a low global warming potential and no ozone-depleting effects [7], making it an important environmental consideration when selecting a working fluid for thermodynamic power generation cycles. When CO_2 approaches its critical point, it becomes less compressible [8]. Consequently, the work required by the compressor can be significantly reduced, leading to improved thermodynamic cycle efficiency. Another advantage of using sCO_2 cycles is that they operate at much higher pressures throughout the cycle, resulting in a higher density of the working fluid, which contributes to smaller equipment sizes, reduced physical footprint, and lower capital expenditures [9].

The authors in [10] conducted a study on sCO_2 waste heat recovery cycles for marine energy systems. The study compared the proposed system, which employs an sCO_2 Brayton cycle, with a conventional Brayton cycle already used for this application. They found that an increase in output power of approximately 18 % could be achieved, along with an overall improvement in onboard energy system efficiency of more than 11 % [11]. A modeling study was conducted to assess the performance improvements of an sCO_2-based preheating system for engine waste heat recovery. The engine under consideration was a six-cylinder turbocharged diesel engine, typical for modern long-haul truck chassis, and suitable for research on ORC waste heat recovery. Simulation results indicate that the enhanced system can better utilize the regeneration heat load and, therefore, improve system performance.

Furthermore, the maximum net engine output with the recovery system was 7.4 % higher than that of the baseline engine. By implementing the improved preheating system, engine power was further increased by 6.9 % [12]. It is also worth noting that a similar study conducted on the same engine using sCO_2-based systems demonstrated an additional increase in engine output power by 8.5 %, highlighting its significant potential for practical application [13].

Organic Rankine Cycle (ORC)

ORC-based waste heat recovery systems have been extensively researched for several decades for application in large-displacement diesel engines. In [14], a comprehensive literature review on ORC research was conducted. The authors found that diesel engines and gas turbines are the most commonly used heat sources for WHR studies.

In [15], a study was conducted on a 10.3-liter, 316 kW turbocharged diesel engine using an ORC WHR system. The system could recover between 2—4 kW at low engine speeds and 8—16 kW at high speeds [16]. In [17], an ORC WHR system was modeled for a Volvo D-13 engine with a displacement of 13 liters and a power output of 367 kW, using a working fluid mixture of 80 % water and 20 % ethanol. It was found that the efficiency of the WHR system ranged from 9 % to 23 %

depending on the waste heat source. The study in [18] examined the performance of ORC for diesel engines of various configurations and found that fuel savings of up to 5 % could be achieved through the effective implementation of ORC systems for engine exhaust gas heat recovery.

In [19], an extensive review of ORC WHR diesel engine research was conducted. It was determined that fuel savings of up to 20 % are realistically achievable, along with thermal efficiency gains of 10—25 % for single-loop ORC systems. These findings were confirmed by the authors of [20], who conducted a similar technical review of compression ignition engines using ORC WHR systems. They found that refrigerant R245fa is the best working fluid for these systems due to its excellent refrigerant properties, availability, and low economic and environmental impact.

Thermoelectric Generators (TEGs)

Thermoelectric processes enable the direct conversion of heat energy into electrical energy. TEGs have great potential for use in waste heat recovery systems in automobiles, heavy machinery, drilling rigs, power plants, and more. They offer several advantages, including low maintenance costs, zero environmental impact, silent operation, compactness, and stability. However, significant technical challenges remain, which have so far limited the progress of these systems. These include low efficiency and low maximum operating temperature, dictated by the choice of thermoelectric materials, as well as integration effects such as increased mass, complexity, and higher exhaust backpressure.

In [21], an experiment was conducted to evaluate the performance and WHR capabilities of TEGs, demonstrating that the power output of TEGs increases with engine load and crankshaft speed. Furthermore, in [22], a maximum power output of 119 W was achieved at 2000 rpm, with a peak conversion efficiency of approximately 8 %. The study in [23] investigated the effect of TEG placement on potential fuel savings in vehicles. It was found that placing the TEG closer to the exhaust manifold could increase fuel savings by up to 20 %.

Formulation of the study purpose

The objective of this study is to assess the potential for electricity recovery using ORC, sCO_2, and TEG systems in waste heat recovery (WHR) systems for the exhaust gases of diesel internal combustion engines (ICEs) used in oil and gas technological transport. This will allow for the determination of their efficiency and suitability for WHR applications.

To achieve this goal, the following tasks have been set:

to develop a diesel engine model in the GT-SUITE software environment;

to design models for TEG, ORC, and sCO_2 systems in GT-SUITE and simulate their interaction with the diesel engine model;

to analyze the obtained results by comparing them with data from scientific literature to determine the most efficient technology for exhaust gas heat recovery in oil and gas technological transport ICEs.

Presenting main material

Modeling Methodology

The study was conducted using GT-SUITE, a specialized software package for simulating engines, transmissions, and vehicles. This software is a powerful tool for modeling various engine systems and is widely used by leading manufacturers in the automotive industry. GT-SUITE includes built-in 3D CAD tools, optimization capabilities, and neural network training options. Additionally, it integrates with MATLAB and Simulink, allowing for more in-depth control system analysis.

An essential part of modeling in GT-SUITE is the calibration of various system components. In this project, the first step was to create standalone calibration models for heat exchangers, compressors, pumps, and turbines used in the diesel engine and WHR system models. These models were compared with reference test data provided by diesel engine manufacturers, as well as other calibration data found in the literature. Once the components were calibrated and the results were validated against test data, modeling for this project commenced.

Modeling of Diesel Engines in the Oil and Gas Industry

For this project, a 6-cylinder, 4-stroke diesel engine with a displacement of 12.0 liters and a compression ratio of 17:1 was used. These are typical engines currently used in various models of oil and gas technology vehicles at PJSC "Ukrnafta".

The heat exchange model in the cylinder used in this study is the WoschniGT model. This model uses a formula that accurately simulates the classic Woschni correlation without turbulence. However, the difference lies in the handling of heat transfer coefficients when the valves are open. The WoschniGT model accounts for heat transfer increased by the intake air velocity through the intake valves, as well as the backflow through the exhaust valves. Additionally, the combustion model used is direct injection (DI), where fuel is injected directly into the cylinder. In this model, the effective engine power is controlled by the amount of fuel injected into the cylinders. Fuel supply is limited in the controller by the air-fuel ratio.

The turbocharger is set to 1 second to reach a constant turbine speed after changes in the engine crankshaft speed. After defining the necessary parameters, the user can input the relevant data required for modeling. The selected values for this project are listed in Tabl. 1.

Table 1. Selected Parameters for the Diesel Engine in Oil and Gas Technology Transport in GT-SUITE

Parameter	Regime 1	Regime 2	Regime 3	Regime 4	Regime 5	Regime 6	Regime 7	Regime 8
Engine power (kW)	240	270	295	305	270	225	155	90
Mass of fuel injected into the cylinders (mg)	255	240	225	210	195	180	165	150
Engine crankshaft speed (rpm)	3000	2400	2000	1800	1600	1400	1200	1000
Turbocharger rotates (rpm)	90 000	86 000	80 000	82 000	77 000	69 000	60 000	52 000

Modeling of the ORC System

In this study, an indirect integration research approach will be adopted. The engine is modeled separately from the WHR model. First, the diesel engine model is developed. After that, the relevant data is inserted into a separate WHR model and simulated to determine the power recovered by the system. This model includes typical components of the ORC system but has the added advantage of utilizing a recuperator, which further enhances the system's efficiency. The working fluid selected for this system is refrigerant R245fa. The choice of working fluid was based on practicality (availability of R245fa and cost).

Modeling of the sCO$_2$ System

Fig. 1 shows the sCO$_2$ system model created in GT-SUITE. The system design is based on a recuperated closed Brayton cycle. This system has the additional advantage of improving overall efficiency through the use of a recuperator. The working fluid for this system is carbon dioxide (CO_2) in a supercritical state. In this state, the temperature and pressure of CO_2 exceed the critical point, making it impossible to distinguish between the liquid and vapor phases. This occurs when the temperature exceeds 31 °C and the pressure is above 83.8 bar.

After modeling the system, the housing configuration section can be determined. The final housing configuration parameters can be seen in Tabl. 2 below. An important parameter is the initial temperature of the refrigerant, which is set at 31 °C to ensure the supercritical state of CO_2 throughout the system.

Modeling of the TEG System

The last system tested in this study is the TEG system. The thermoelectric modules (TEM) included in the TEG system are shown in Fig. 2.

Each tube is modeled as a "flat plate," similar to those found in a typical plate heat exchanger. The tubes are simulated using heat pipes connected to masses that represent the tube walls and fins for the inner tube.

Additionally, the TEM template used in the model accounts for all three thermoelectric effects (Seebeck, Peltier, and Thomson) to generate electrical potential based on the temperature difference across it. The same process is repeated for all 10 TEMs to create a complete model.

To analyze the power generated by the entire TEG system, a submodel was created to sum up all the output power from each TEM. The TEG configuration parameters are presented in Tabl. 2.

Table 2. Final selected parameters for the TEG model in GT-SUITE

Parameter	Regime 1	Regime 2	Regime 3
Mass flow of coolant (kg/s)	0,1	0,4	0,8
Mass flow of exhaust gases (kg/s)	0,13693	0,32345	0,47707
Coolant outlet pressure (MPa)	0,1	0,1	0,1
Exhaust pressure at the outlet (MPa)	0,1009656	0,10482228	0,10881422
The temperature of the coolant at the inlet (°C)	25	25	25
Exhaust temperature at the inlet (K)	655,5935	711,7872	783,91376

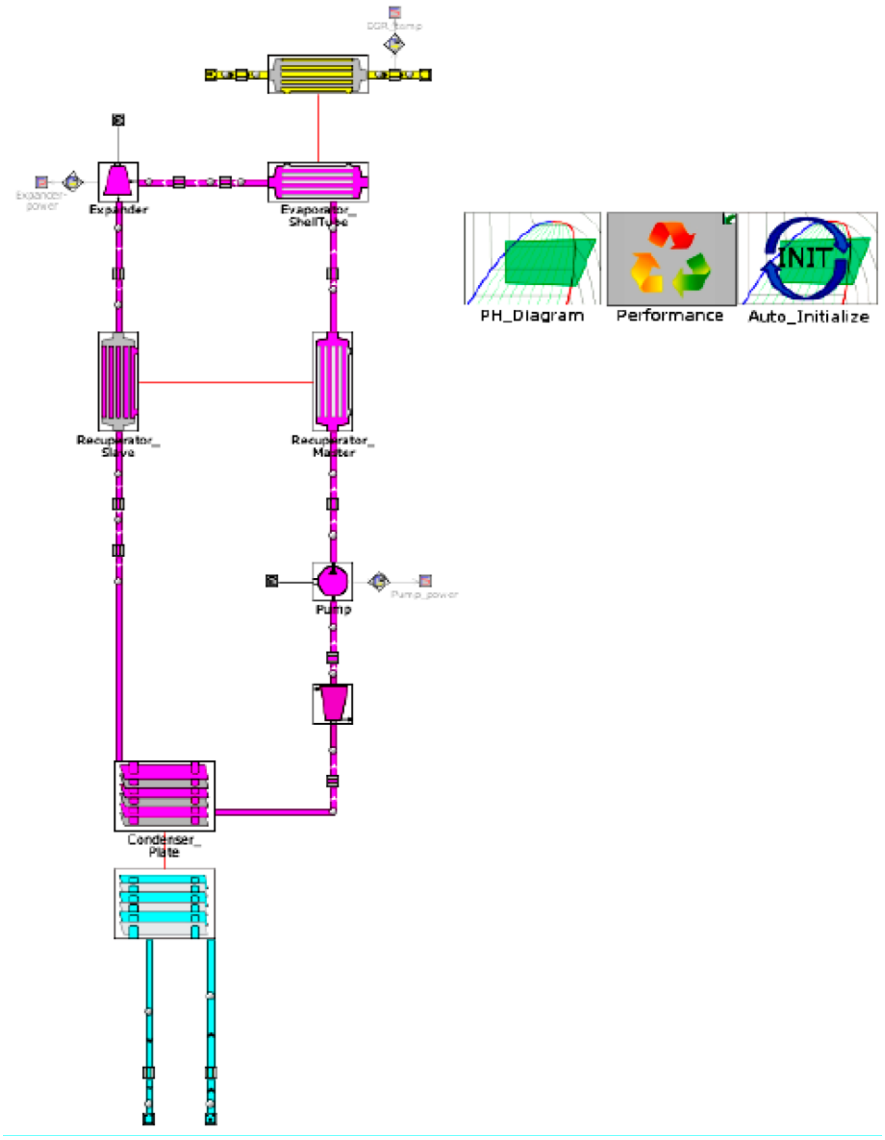

Fig. 1. Schematic of the sCO2 system model in GT-SUITE

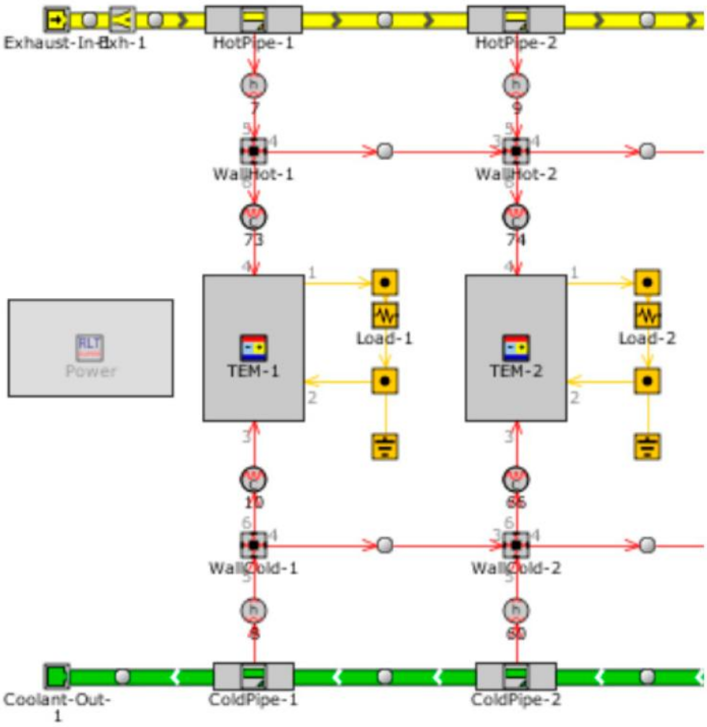

Fig. 2. Scheme of the TEG system

Results and Discussion

After modeling the diesel engine and waste heat recovery systems, the corresponding simulation results of the diesel engine were analyzed.

In Fig. 3, the brake torque generated by the engine within the same RPM range can be observed. We can see that the maximum brake torque is approximately 1540 N·m at 1400 RPM. Once again, this value is representative of current production high-power diesel engines within this power range, further increasing confidence in the model.

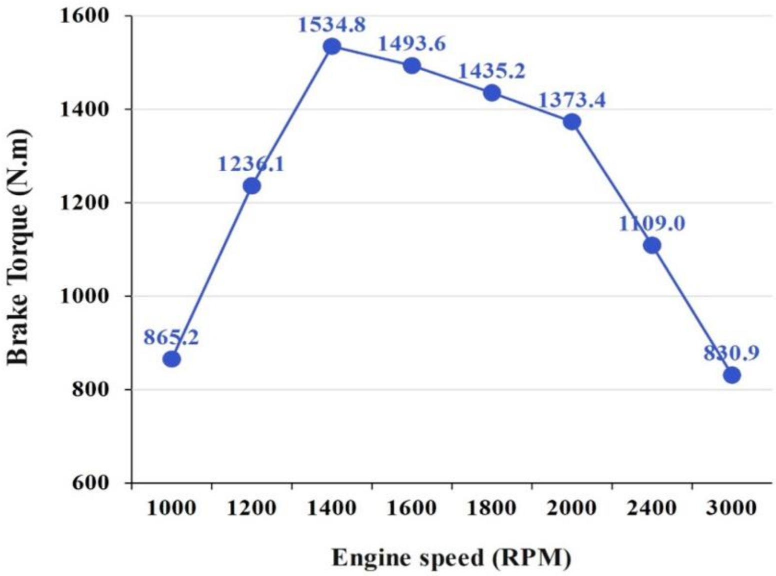

Fig. 3. The dependence curve of engine torque (N·m) from the crankshaft rotation frequency (rpm)

After obtaining the power and torque curves from the engine, it is essential to select several operating modes to study the amount of power that the WHR system can recover during typical NGT engine operating scenarios.

In this project, three operating modes were selected:

Regime **1:** Low power and torque point (90 kW) — 1000 RPM was chosen as an additional point of interest.

Regime **2:** Maximum torque point (225 kW) — 1540 N·m was generated at 1400 RPM.

Regime **3:** Maximum power point (305 kW) — the model produces 305 kW at 1800 RPM.

Fig. 4 illustrates the mass flow rate of exhaust gases at the selected points of interest (1000 RPM, 1400 RPM, and 1800 RPM). These values, along with the exhaust temperature values at the test points shown in Fig. 5, were used as input exhaust parameters in the WHR models. After obtaining these exhaust values, an indirect approach was applied, as discussed in the "Methodology" section of the report.

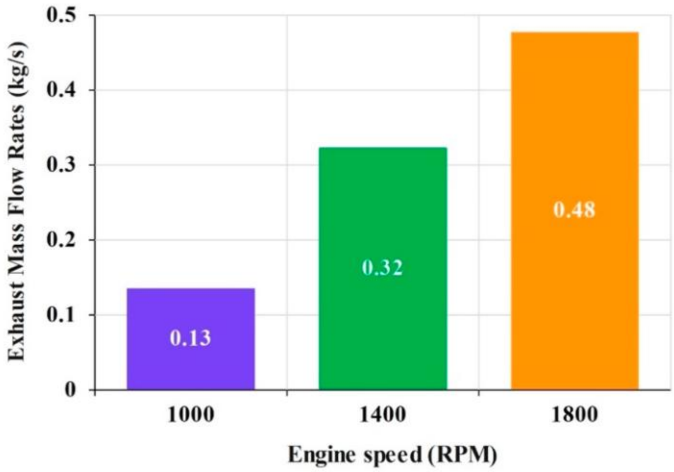

Fig. 4. Mass flow of exhaust gases for selected points of interest

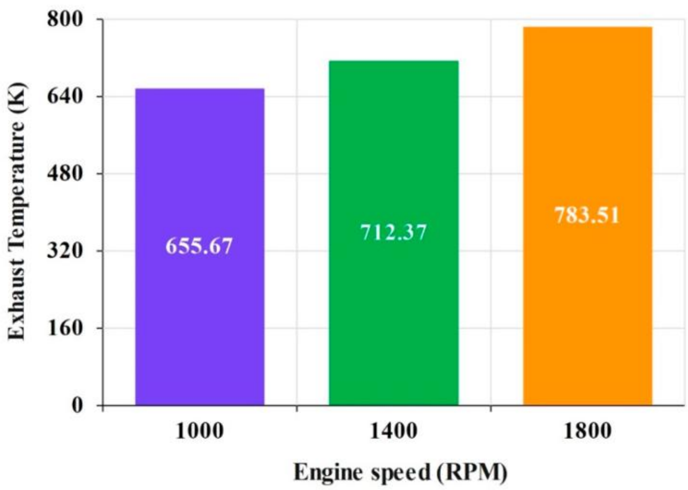

Fig. 5. Exhaust temperature for selected points

Processing Results

Overall, based on the results of all three WHR systems, Fig. 6 shows that the most promising systems for successfully applying exhaust gas waste heat recovery in heavy-duty diesel engines are the ORC and sCO_2 systems. These two systems have significantly higher efficiency than the TEG system and therefore recover much more energy from the exhaust gases.

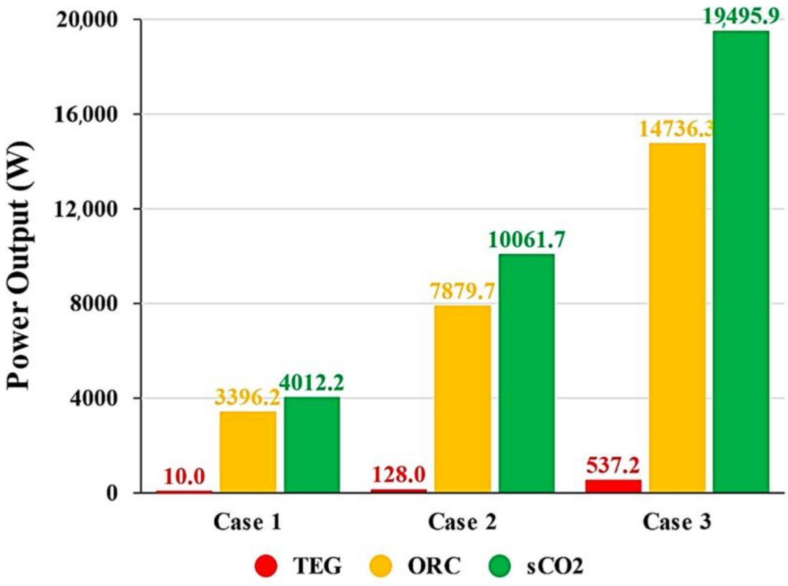

Fig. 6. Comparison of three WHR systems

Additionally, sCO_2 systems have the added advantage of being more compact due to the higher operating pressure of the system. However, the main challenge faced by both ORC and sCO_2 systems is the development of highly efficient turbines that remain reliable under increased pressures and temperatures. If these challenges can be overcome, there is significant potential for the widespread adoption of these systems in WHR applications.

This study is the only one that examines all three major heat recovery systems for mobile applications. Previous studies discussed in the literature (see [34]) have not addressed the implementation of sCO_2. Therefore, the value of this research lies in the simultaneous evaluation of these three primary waste heat recovery options within a single study, based on a common comparative framework.

Conclusions

The objective of this study was to explore the potential of ORC, sCO_2, and TEG systems for utilization in diesel engines of oil and gas technology transport to recover exhaust gas energy. Various simulations and experimental studies have been conducted on these systems for different applications; however, they have not yet been widely adopted in transportation.

Based on the obtained results, it can be confidently stated that sCO_2 and ORC systems are the most viable candidates for WHR applications in diesel engines. Among the three WHR systems, sCO_2 exhibits the highest efficiency and offers the additional advantage of compactness due to its higher operating pressure. Moreover, the cost per kW of electricity generated by sCO_2 systems is significantly lower than that of ORC and TEG systems.

Of course, the applicability of such systems remains a topic of debate in the context of transportation electrification. However, the increasing adoption of alternative fuels and hydrogen-based solutions suggests that these systems can be reconsidered with renewed interest. It is evident that some challenges still need to be addressed regarding component design and system availability for mass production. Nonetheless, if these challenges are overcome, the potential of these systems could be utilized in the near future. The energy recovered by these systems can be used to power auxiliary components such as air conditioning or lighting, thereby reducing vehicle fuel consumption. Given the growing pressure on automotive manufacturers to reduce emissions from their vehicles, these WHR systems could present an attractive prospect.

In industrial applications, sCO_2 and ORC systems will require higher maintenance demands compared to TEG systems. However, in the context of transportation, these maintenance requirements are likely to be minimal by design, although evaluating this aspect falls beyond the scope of this study.

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