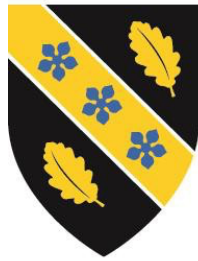


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***Mathematical Principles of Thermodynamics
Applied to Ideal Gases and Heat Engines and
their cycles.***

ACMA5011 – Thermo-fluid Mechanics

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Table of Contents

1.0 Executive Summary	2
2.0 Introduction.....	3
3.0 Part A	4
4.0 Part B – Ideal Carnot Heat Engine	11
5.0 Part C	14
6.0 Conclusion.....	17
7.0 Bibliography.....	18

1.0 Executive Summary

This report analyses several aspects of thermodynamics principles that apply to ideal gases and heat engines. This includes the application of the first and second laws of thermodynamics. The report identifies several key findings that relate to theoretical models within stated assumptions throughout.

Part A focuses on the ideal gas behaviour, using ideal gas theory equation and kinetic theory. This is to undertake calculations in molecular quantities, pressures, and internal energy changes. With full comprehensive steps in calculations, the analysis includes systems involving temperature, volume gradients, and conservations of mass and energy in closed systems.

Part B describes the concept used for the ideal 'Carnot' heat engine, used as an example of maximum efficiency from a theoretical perspective. Mathematical calculations along with conceptual diagrams were used to analyse isothermal and adiabatic expansion and compression in thermodynamic processes.

The final section, Part C, differs from the previous sections by introducing real-gas corrections, using theories such as van der Waals equation and Graham's Law of diffusion. Kinetic theory is considered throughout to demonstrate the relationship between pressure, molecular speed, density, and temperature.

2.0 Introduction

Thermodynamics is a key discipline in energy and mechanical engineering. Understanding the behaviour and characteristics of various molecules and gases play a vital role in producing effective engineering solutions. The fundamental principles of thermodynamics convey knowledge in heat transfer, conservation of energy, and other formula ensure their use in predicting behaviours and characteristics of gases in various industry tasks, such as engines, refrigeration, power plants, along with so many others.

The use of ideal gas laws allows for advanced considerations of gas' characteristics at a quantitative state, where fewer considerations and external factors require consideration. This means that calculations can be stripped down to key principles in theoretical thermodynamics.

This is shown most clearly in Part B of the report, highlighting how the Carnot engine's idealistic model can be used as a high-level target for developers of the technology. The Second law of Thermodynamics limits the ability for practical results for industry use, therefore the assumptions and limitations of the law are identified and challenged.

Limitations of the ideal gas model is assisted with the use of real gas behaviour, along with kinetic theory formulas. The report demonstrates the impact of molecular behaviour at a microscopic level and its impact of engineering design and performance.

The laws of thermodynamics, being that energy can never be created or destroyed, only transferred, and the total disorder of a system can never decrease over time, remains the key laws that must be considered throughout the entirety of the report. Without considering these laws, key assumptions and observations made that do not conform to these laws become negligible.

3.0 Part A**1) (i) Number of moles**

$$\begin{aligned}
 n &= \frac{PV}{RT} \\
 &= \frac{(1.5 \times 10^6) \times (8.0 \times 10^{-3})}{(8.31) \times (400.15)} \\
 &= \frac{1.2 \times 10^4}{3325.25} \\
 &= 3.61 \text{ mol}
 \end{aligned}$$

(ii) Number of molecules

$$\begin{aligned}
 N &= nN_A \\
 &= (3.61) \times (6.023 \times 10^{23}) \\
 &= 2.17 \times 10^{24} \text{ molecules}
 \end{aligned}$$

(iii) Mass of one molecule

$$\begin{aligned}
 m_{\text{molecule}} &= \frac{M}{N_A} \\
 &= \frac{32 \times 10^{-3}}{6.023 \times 10^{23}} \\
 &= 5.31 \times 10^{-26} \text{ kg}
 \end{aligned}$$

2) Two connected bulbs at different temperatures

$$\begin{aligned}
 n_{\text{total}} &= \frac{P_0(V_A + V_B)}{RT_0} \\
 &= \frac{(1.0 \times 10^5) \times (3.0 \times 10^{-3})}{(8.31) \times (273)} \\
 &= \frac{300}{2268.63} \\
 &= 0.132 \text{ mol}
 \end{aligned}$$

$$n_{total} = \frac{PV_A}{RT_A} + \frac{PV_B}{RT_B}$$

$$P = \frac{n_{total}R}{\frac{V_A}{T_A} + \frac{V_B}{T_B}}$$

$$P = \frac{(0.132) \times (8.31)}{\frac{2.0 \times 10^{-3}}{500} + \frac{1.0 \times 10^{-3}}{273}}$$

$$P = 1.43 \times 10^5 Pa$$

Molecular impacts on a cube face

Time between collision on two parallel faces

$$t = \frac{L}{v}$$

$$t = \frac{1}{500}$$

$$t = 2.0 \times 10^{-3} s$$

Change in momentum on a face for one molecule

$$\Delta p = 2mv$$

$$\Delta p = 2 \times (5.0 \times 10^{-26}) \times (500)$$

$$\Delta p = 5.0 \times 10^{-23} kgms^{-1}$$

Total force on that face

$$Nf = \frac{N}{3}$$

$$Nf = 3.0 \times 10^{24}$$

$$t_{return} = \frac{2L}{v}$$

$$t_{return} = \frac{2}{500}$$

$$t_{return} = 4.0 \times 10^{-3} s$$

$$f = \frac{1}{t_{return}}$$

$$f = 250 \text{ s}^{-1}$$

$$N_{total} = N_f f$$

$$N_{total} = (3.0 \times 10^{24}) \times (250)$$

$$N_{total} = 7.5 \times 10^{26} \text{ s}^{-1}$$

$$F = N_{total} \Delta p$$

$$F = (7.5 \times 10^{26}) \times (5.0 \times 10^{-23})$$

$$F = 3.75 \times 10^4 \text{ N}$$

Pressure on the face

$$P = \frac{F}{A}$$

$$P = \frac{3.75 \times 10^4}{1}$$

$$P = 3.75 \times 10^4 \text{ Pa}$$

Isothermal compression then adiabatic expansion

$$P_2 = P_1 \frac{V_1}{V_2}$$

$$P_2 = 2.0 \times 10^6 \times 3$$

$$P_2 = 6.0 \times 10^6 \text{ Pa}$$

Adiabatic expansion $PV^r = \text{constant}$

$$P_3 = P_2 \left(\frac{V_2}{V_3} \right)^r$$

$$P_3 = 6.0 \times 10^6 \left(\frac{1/3}{1} \right)^{1.3}$$

$$P_3 = 6.0 \times 10^6 (3^{-1.3})$$

$$\begin{aligned}
 3^{1.3} &= e^{1.3 \ln 3} \\
 e^{1.3(1.0986)} &= e^{1.428} \\
 4.17 &= 3^{-1.3} \\
 &= 0.240
 \end{aligned}$$

$$\begin{aligned}
 P_3 &= 6.0 \times 10^6 (0.240) \\
 P_3 &= 1.44 \times 10^6 \text{ Pa}
 \end{aligned}$$

First law: internal energy change

Given $Q = 800J$ added to gas, work done by gas $W = 375J$.

$$\begin{aligned}
 \Delta U &= Q - W \\
 800 - 375 &= 425J \\
 \Delta U &= +425J
 \end{aligned}$$

Carnot engines with equal efficiency

Carnot efficiency

$$\eta = 1 - \frac{T_C}{T_H}$$

Case a: $T_H = 1000 \text{ K}, T_C = 500 \text{ K}$

$$\begin{aligned}
 \eta &= 1 - \frac{500}{1000} \\
 \eta &= 0.5
 \end{aligned}$$

Case b: between 300 K and $T \text{ K}$.

$$\begin{aligned}
 \text{So } T_H &= T, T_C = 300 \\
 0.5 &= 1 - \frac{300}{T}
 \end{aligned}$$

$$\begin{aligned}
 T &= \frac{300}{0.5} \\
 T &= 600 \text{ K}
 \end{aligned}$$

3) Maximum efficiency of a Carnot-type engine from heat flows

Given $Q_H = 10,000 J$, $Q_C = 2,000 J$

$$\eta_{total} = 1 - \frac{Q_C}{Q_H}$$

$$\eta_{total} = 1 - \frac{2000}{10000}$$

$$\eta_{total} = 0.8$$

$$\eta_{total} = 80\%$$

4) Entropy changes of water heated reversibly

Given: $m = 10kg$, $C_p = 4.20 \times 10^3 J kg^{-1} K^{-1}$

$T_1 = 373 K$, $T_2 = 573 K$

$$\Delta S = mC_p \ln\left(\frac{T_2}{T_1}\right)$$

$$\Delta S = (10) \times (4.20 \times 10^3) \times \ln\left(\frac{573}{373}\right)$$

$$\Delta S = 42000 \ln(1.536)$$

$$\ln(1.536) = 0.430$$

$$\Delta S = 42000(0.430)$$

$$\Delta S = 1.80 \times 10^4 J K^{-1}$$

5) Change in Internal Energy

Given: Heat supplied to the gas: $Q = +800 J$. Work done by the gas: $W = +375 J$

The cylinder is well lagged and the piston is frictionless.

$$\Delta Q = \Delta_u + \Delta_w$$

$$800 = \Delta_u + 375$$

$$800 - 375 = \Delta_u$$

$$\Delta u = 425$$

$$\Delta u = 425 J$$

Question 6 – Carnot Engine Efficiency

Case A: Hot reservoir temperature - $T_1 = 1000 K$, Cold reservoir temperature - $T_2 = 500 K$

Case B: Hot reservoir temperature - $T_4 = 300 K$, Cold reservoir temperature - $T_3 = T K$

$$\eta = 1 - \frac{T_2}{T_1}$$

Case A:

$$\eta_A = 1 - \frac{500}{1000} = 1 - 0.5 = 0.5$$

Case B:

$$\eta_B = 1 - \frac{300}{T}$$

$$\eta_A = \eta_B :$$

$$0.5 = 1 - \frac{300}{T}$$

$$\frac{300}{T} = 0.5$$

$$T = \frac{300}{0.5}$$

$$T = 600 K$$

$$T = 600 K$$

Question 7 – Maximum Efficiency of a Carnot Heat Engine

Given:

Heat absorbed from the source: $Q_1 = 10,000 \text{ J}$

Heat rejected to the sink: $Q_2 = 2,000 \text{ J}$

Maximum efficiency

$$\eta = \left(1 - \frac{Q_2}{Q_1}\right) \times 100$$

$$\eta = \left(1 - \frac{2,000}{10,000}\right) \times 100$$

$$\eta = 80$$

$$\eta = 80 \%$$

Question 8 – Change in Entropy

$$\Delta S = \int_{T_1}^{T_2} m C_w \frac{dT}{T}$$

$$\Delta S = m C_w \int_{T_1}^{T_2} \frac{dT}{T}$$

$$\Delta S = m C_w [\ln(T)]_{273}^{573}$$

$$\Delta S = 10 \times 4.2 \times 10^3 \times [\ln(573) - \ln(273)]$$

$$\Delta S = 18030.91$$

$$\Delta S = 18.0 \times 10^3 \text{ J K}^{-1}$$

4.0 Part B – Ideal Carnot Heat Engine

A Carnot heat engine differs to similar innovations in its ability to work reversible between a hot reservoir at T_H and a cold reservoir at T_C . Its innovation is effective as it defines an upper theoretical limit for efficiency. This means that no engine between the same two temperatures as the reservoirs can be more efficient than the Carnot heat engine. As legislation and changes in environmental policies worldwide adapt, efficiency in heat transfer and collection is one of the most desirable assets to organisations in the manufacturing and engineering industries. Using the ideal model of the Carnot engine inspires innovation in the recycling of energy that manufacturers can follow, with data to accompany any idealisations and assumptions made in energy retention. (Feidt, 2020).

Engine flow:

Heat in from T_H : Q_H

Work out: W_{net}

Heat rejected to T_C : Q_C

$$Q_H = W_{net} + Q_C$$

Carnot cycle process

The Carnot heat engine cycle is defined by four primary processes, all of which are reversible for an ideal gas working fluid.

1. Isothermal Expansion – T_H

Gas absorbs heat from source Q_H and works whilst the temperature is consistent with that at T_H .

2. Adiabatic Expansion

With this process, no heat transfer occurs, only a drop in temperature from that of source T_H to T_C .

3. Isothermal compression – T_C

Heat is rejected at source Q_C at a constant cold temperature.

4. Adiabatic compression

With the final process of the four, no heat transfer occurs, with the temperature rising from T_C , returning to temperature at the first process of T_H .

Efficiency derivation

Reversible Carnot Engine:

$$\eta = \frac{W_{net}}{Q_H} = 1 - \frac{Q_C}{Q_H}$$

Reversibility implies:

$$\frac{Q_H}{T_H} = \frac{Q_C}{T_C} \rightarrow \frac{Q_C}{Q_H} = \frac{T_C}{T_H}$$

Therefore:

$$\eta_{Carnot} = 1 - \frac{T_C}{T_H}$$

The efficiency calculated is dependent on the reservoir temperatures; it does not consider working fluid temperature. In a practical application, the working fluid temperature would influence several aspects of the process, such as fluid density, molecular speed, and gas behaviour. (*Feidt, 2020*).

The Carnot's efficiency is unique to the design of the system, showing differences between its use and real engines. Real engines are less efficient due to the lack of reversibility that is available in Carnot engines. The concept adheres to laws of thermodynamics, showing basic adherence to principles that underpin all research and development in the research of energy storage and conversion systems.

Examples of considerations are:

- Friction; between the piston, shaft, and bearings.
- Finite temperature differences needed for heat transfer; Without this larger risk of failure and entropy occur within the system.
- Pressure differences in valves, heat exchangers.
- Non-quasi static processes.
- Heat losses and imperfect insulation.
- Material limits (max T_H) and environmental limits (min T_C).

The reasons listed above show why the Carnot engine is a benchmark and does not correlate to a practical design for industry use.

Heat Pumps and Refrigeration comparison

A heat pump and refrigerator are a variation of the process used for the Carnot cycle, only reversed. In this scenario, work is used to move heat from hot to cold, which does not contradict the second law as external work input is required. Whilst the Carnot engine's goal is to produce work from heat, this differs from a refrigerator, where its main performance aim is to move heat to cold.

Refrigerator: desired output Q_C (cooling)

$$COP_R = \frac{Q_C}{W_{in}}$$

Heat pump: desired output Q_H (heating)

$$COP_{HP} = \frac{Q_H}{W_{in}}$$

As $Q_H = Q_C + W_{in}$:

$$COP_{HP} = COP_R + 1$$

Carnot COP limits:

$$COP_{R,Carnot} = \frac{T_C}{T_H - T_C}, \quad COP_{HP,Carnot} = \frac{T_H}{T_H - T_C}$$

5.0 Part C

Ideal gas

- Terms of an ideal gas molecules behaviour:
- Occupy negligible volume
- Exert no intermolecular forces
- Collide elastically
- Exhibit random motion

(Kivi, 2020).

Equation of state

$$PV = nRT$$

Molecular form

$$PV = NkT$$

$$k = R/N_A$$

The limitations of this are that when real gases are subject to high pressure and low temperature, they deviate due to finite molecular size and attractive forces.

Real-gas correction: Van der Waals equation

$$\left(P + a \left(\frac{n}{V}\right)^2\right)(V - nb) = nRT$$

Terms:

- $V - nb$: free volume correction. Molecules have finite size. b refers to excluded volume.
- $P + a(n/V)^2$: pressure correction due to intermolecular attractions reducing wall impact pressure. The actual pressure is therefore lower, which requires the correction to be added back.
- a quantifies attraction strength; b quantifies molecular size.

Kinetic theory

Based on findings in kinetic theory, pressure arises from molecular impacts. For N molecules of mass m in volume V , with mean square speed c^2 .

$$P = \frac{1}{3} \frac{N}{V} mc^2$$

Multiply by V .

$$PV = \frac{1}{3} Nmc^2$$

Ideal gas law in molecular form:

$$PV = NkT$$

$$NkT = \frac{1}{3} Nmc^2 \rightarrow kT = \frac{1}{3} mc^2$$

$$Ek = \frac{1}{2} mc^2 = \frac{3}{2} kT$$

$$Ek \propto T$$

Constant pressure C_{rms} inversely proportional to density

Define root mean square speed:

$$C_{rms} = \sqrt{C^2}$$

From kinetic pressure relation:

$$P = \frac{1}{3} \rho c_{rms}^2$$

Because

$$\rho = \frac{Nm}{V}$$

Rearrange for C_{rms} :

$$C_{rms} = \sqrt{\frac{3P}{\rho}}$$

At constant P :

$$C_{rms} \propto \frac{1}{\sqrt{\rho}}$$

Grahams Law of diffusion

When temperature and pressure remain constant, ideal-gas density is proportional to molar mass.

$$\rho = \frac{RM}{RT} \rightarrow \rho \propto M \quad (P, T \text{ constant}).$$

Using constant P

$$C_{rms} \propto \frac{1}{\sqrt{\rho}}$$

$$C_{rms} \propto \frac{1}{\sqrt{M}}$$

r is proportional to molecular speed:

$$\frac{r_1}{r_2} = \sqrt{\frac{M_2}{M_1}}$$

Graham's Law is used for gas mixture separation. Using the law, the gas behaviour is idealised with being dilute gas and a negligible intermolecular force. (*Çengel, Boles and Kanoglu, 2019*).

6.0 Conclusion

The report has showcased the theoretical and practical application of thermodynamic principles, in both gas and energy examples. The basis of several theories such as ideal gas laws, kinetic energy, and the First law of Thermodynamics has been used in solutions to theoretical variables and solutions. The analysis of these theories displayed how the molecular motion and energy exchange directly impacted macroscopic properties such as pressure and temperature.

The analysis of the Carnot engine provided insight into the factors that limits cyclic processes from the Second Law of thermodynamics. Findings in this section highlighted the crucial variable of reservoir temperature in the efficiency of such systems, where sudden temperature changes will dramatically effect energy transfer in the application. Comparisons in this section with refrigerating and heat pumps provided further insight into how work input enable heat transfer within previously stated thermodynamic laws.

The third and final section of the report evaluated the assumptions and calculations imposed by ideal-gas theories by comparing the real gas theories with that of real-gas behaviour. Van der Waals, along with kinetic theory and Graham's law, considered the behaviour of molecular size and forces, as well as the expressions to link molecular size with density and speed.

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