Chapter Four

Thermodynamic Modeling

4.1. INTRODUCTION

In this chapter we will address the thermodynamic model for Joule-Brayton cycle, and we will take into account the change in the specific heat values of the working substance due to change in temperature. We will use MATLAB software to create a program to conduct the thermodynamic model calculations, and then we will present the results that will be obtained when we execute the program.

4.2. JOULE-BRAYTON CYCLE THERMODYNAMIC CYCLE MODEL

Thermodynamic cycle model for Joule-Brayton cycle consist of four processes as shown in fig. 4.1 as follow.



Fig. 4.1: T-s diagram of an air standard Joule-Brayton cycle model.

Process $1 \rightarrow 2s$ is a reversible adiabatic process or isentropic compression process, while process $1 \rightarrow 2$ is an irreversible adiabatic compression process that takes into account the internal irreversibility in

the real compression process. Process $2 \rightarrow 3$ is a constant pressure heat addition or an isobaric heat addition. Process $3 \rightarrow 4s$ is a reversible adiabatic expansion process or isentropic expansion process, while process $3 \rightarrow 4$ is an irreversible adiabatic expansion process that takes into account the internal irreversibility in the real expansion process. Process $4 \rightarrow 1$ is a constant pressure heat rejection process or an isochoric heat rejection process.

4.3. THERMODYNAMIC MODEL ANALYSIS

In most cycle's models, the working fluid is assumed to be having as an ideal gas with constant specific heats. But this assumption can be valid only for small temperature difference. For the large temperature difference encountered in realistic cycle, this assumption cannot be applied.

According to reference [12], for the temperature range of 200-1000 K, the specific heat of air at constant pressure can be written as:

 $C_p = 2.506 \times 10^{-11}T^2 + 1.454 \times 10^{-7}T^{1.5} - 4.246 \times 10^{-7}T \\ + 3.162 \times 10^{-5}T^{0.5} + 1.3303 - 1.512 \times 10^4T^{-1.5} + 3.063 \times 10^5T^{-2} \\ - 2.212 \times 10^7T^{-3} \end{pmatrix} \dots (4-1)$

Where:

 $C_p \equiv$ The constant pressure specific heat (kJ/kg.K).

 $T \equiv$ The temperature of air (K).

According to the relation between constant pressure specific heat and constant volume specificheat:

$$C_p - C_v = R \dots \dots \dots (4-2)$$

Where:

 $R \equiv$ The gas constant of the air and equal [0.2883] (kJ/kg.K).

The constant volume specific heat can be written as follow:

$$C_{v} = C_{p} - R = 2.506 \times 10^{-11}T^{2} + 1.454 \times 10^{-7}T^{1.5} - 4.246 \times 10^{-7}T + 3.162 \times 10^{-5}T^{0.5} + 1.0433 - 1.512 \times 10^{4}T^{-1.5} + 3.063 \times 10^{5}T^{-2} + 2.212 \times 10^{7}T^{-3}$$

Where:

 $C_{v} \equiv$ The constant volume specific heat (kJ/kg.K).

Equations (4 - 1) and (4 - 3) is based on the assumption that air isan ideal gas mixture containing 78.09% nitrogen, 20.95% oxygen, 0.93% argon, and 0.03% carbon dioxide (on mole basis).

Actually, we find that the specific heat of the elements that compose the air has different degree of dependence on temperature. Some elements specific heats arestrongly dependent on temperature, while others are less dependent. Thus, it is more accurate tocalculate the specific heat of the mixture as a summation of individual elements specific heats.

The temperature-dependent specific heat at constant pressure for the elements that compose the air takes the general form (reference [13]):

$$\frac{C_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \dots \dots \dots (4-4)$$

Where:

 $R \equiv$ The gas constant of the element (kJ/kg.K).

 $a_1, a_2, \dots a_5 \equiv \text{Constants.}$

The constants in equation (4 - 4) are given in tables (4 - 1) (a) and (4 - 1) (b) for the elements that compose the air in addition to the gases that appear as combustion products.

i	Species	a_1	a_2	a_3	a_4	a_5
1	CO_2	0.24007797E+01	0.87350957E-02	-0.66070875E-05	0.20021861E-08	0.63274039E-15
2	H ₂ O	0.40701275E+01	-0.11084499E-02	0.41521180E-05	-0.29637404E-08	0.80702103E12
3	N_2	0.36748261E+01	-0.12081500E-02	0.23240102E-05	-0.63217559E-09	-0.22577253E-12
4	O ₂	0.36255985E+01	-0.18782184E-02	0.70554544E-05	-0.67635137E-08	0.2155593E-11
5	CO	0.37100928E+01	-0.16190964E-02	0.36923594E-05	-0.20319674E-08	0.23953344E-12
6	H ₂	0.30574451E+01	0.26765200E-02	-0.58099162E-05	0.55210391E-08	-0.18122739E-11

Table 4.1(a): Coefficients for species temperature-dependent specific heats $[T \le 1000 K]$.

Table 4.1(b): Coefficients for species temperature-dependent specific heats [1000 < T < 3200 K].

i	Species	a_1	a_2	<i>a</i> ₃	a_4	<i>a</i> ₅
1	CO_2	0.446080E+01	0.309817E-02	-0.123925E-05	0.227413E-09	-0.155259E-13
2	H ₂ O	0.271676E+01	0.294513E-02	-0.802243E-06	0.102266E-09	-0.484721E-14
3	N2	0.289631E+01	0.151548E-02	-0.572352E-06	0.998073E-10	-0.652235E-14
4	O ₂	0.362195E+01	0.736182E-03	-0.196522E-06	0.362015E-10	-0.289456E-14
5	CO	0.298406E+01	0.148913E-02	-0.578996E-06	0.103645E-09	-0.693535E-14
6	H ₂	0.310019E+01	0.511194E-03	0.526442E-07	-0.349099E-10	0.369453E-14

In this study we will assume that the air consists of 76.7% nitrogen and 23.3% oxygen (on mass basis).

To calculate the values of gas constant for the above gases we must know the values of molecular weight of these gases as shown in Table (4-2).

Table 4.2: Molecular weight of air constituent gases

	constituent	M (kg/kmol)
1	N_2	28
2	O_2	32

Generally, the specific heat at constant pressure for mixture of gases can be obtained as follow:

$$C_p = \sum_{i=1}^n x_i C_{p_i} \quad \dots \dots \dots \dots \dots (4-5)$$

Where:

 $C_{p_i} \equiv$ The specific heat at constant pressure for component *i* (kJ/kg.K). x_i \equiv The mass fraction for component *i*.

Also, the gas constant for mixture of gases can be obtained as follow:

$$R = \sum_{i=1}^{n} \frac{x_i R_u}{M_i} \qquad \dots \dots \dots \dots (4-6)$$

Where:

 $R_u \equiv$ The universal gas constant [8.3145] (kJ/kmol.K).

 $M_i \equiv$ The molecular weight for component *i* (kg/kmol).

Finally, the molecular weight for mixture of gases can be obtained as follow:

$$M = \sum_{i=1}^{n} y_i M_i \quad \dots \dots \dots (4-7)$$

Where:

 $M_i \equiv$ The molecular weight for component *i* (kJ/kg.K).

 $y_i \equiv$ The mole fraction for component *i*.

The mole and the mass fractions for the fuel are given respectively by the following equations:

Where:

 $n_a \equiv$ Number of moles of air (kmol).

The mole and the mass fractions for the air are obtained respectively by the following equations:

The power consumed by compressor and the power produced by turbine can be calculate as follow:

$$\dot{W}_{C} = \dot{m}_{a}C_{p_{a}}(T_{2} - T_{1}) \dots \dots (4 - 12)$$

 $\dot{W}_{T} = (\dot{m}_{a} + \dot{m}_{f})C_{p_{mix}}(T_{3} - T_{4}) \dots \dots (4 - 13)$

Where:

 $C_{p_a} \equiv$ Specific heat at constant pressure for air (kJ/kg.K). $C_{p_{mix}} \equiv$ Specific heat at constant pressure for products (kJ/kg.K). $\dot{m}_a \equiv$ The mass flow rate of air (kg/s). $\dot{m}_f \equiv$ The mass flow rate of fuel (kg/s). For adiabatic compression (process $1 \rightarrow 2$) and adiabatic expansion(process $3 \rightarrow 4$), the isentropic efficiency for compressor and turbine can be defined asfollow:

$$\eta_c = \frac{T_{2s} - T_1}{T_2 - T_1} \qquad \dots \dots \dots (4 - 14)$$
$$\eta_T = \frac{T_3 - T_4}{T_3 - T_{4s}} \qquad \dots \dots \dots (4 - 15)$$

These two efficiencies can be used to describe the internal irreversibility of the processes.

Since the values of the specific heats $(C_p \text{and} C_v)$ depends on the temperature, adiabatic exponent $\gamma = \frac{C_p}{C_v}$ will vary with temperature as well. Therefore, the equation often used in reversible adiabatic process or isentropic process with constant γ cannot be used in isentropic process with variable γ . A suitable engineering approximation has been utilized for reversible adiabatic process with variable γ . Any reversible process between *i* and *j* has considered a large numbers of infinitesimally small processes with constant γ . In that case infinitesimally small change in temperature dT and pressure dP of the working fluid takes place which may be represented as follow:

With Newton's binomial of right side of equation (4 - 16) and betake the small amounts, yields the fallowing relation:

$$(T+dT)P^{\frac{\gamma-1}{\gamma}}=T\left(P^{\frac{\gamma-1}{\gamma}}+\frac{\gamma-1}{\gamma}P^{\frac{-1}{\gamma}}dP+\cdots\right)\dots(4-17)$$

By rearranging the equation (4 - 17), we get:

By dividing the equation (4-2) on C_p we get:

$$1 - \frac{C_v}{C_p} = \frac{R}{C_p} \qquad or \qquad \frac{\gamma - 1}{\gamma} = \frac{R}{C_p} \qquad \dots \dots \dots (4 - 19)$$

Substituting $\left(\frac{\gamma-1}{\gamma}\right)$ into equation (4 – 18) and rearrange it, yields fallowing relation:

By integrating the equation (4 - 20) between *i* and *j* we get:

$$\int_{i}^{j} R \frac{dP}{P} = \int_{i}^{j} C_{p} \frac{dT}{T} \qquad \rightarrow \qquad R \ln \frac{P_{j}}{P_{i}} = C_{p} \ln \frac{T_{j}}{T_{i}} \dots (4-21)$$

Where the temperature in equation of C_p is logarithmic mean temperature (LMT) for process $i \rightarrow j$:

$$LMT_{i \to j} = \frac{T_j - T_i}{\ln \frac{T_j}{T_i}} \dots \dots \dots (4 - 22)$$

The pressure ratios for Joule-Brayton cycle are defined as follow: Pressure ratio:

$$r_p = \frac{P_2}{P_1} \dots (4-23)$$

We can reformulate the equation (4 - 21) for reversible compression process $(1 \rightarrow 2s)$ and reversible expansion process $(3 \rightarrow 4s)$ respectively as follow:

$$R \ln r_p = C_p \ln \frac{T_{2s}}{T_1} \dots (4 - 24)$$
$$R \ln \left(\frac{1}{r_p}\right) = C_p \ln \frac{T_{4s}}{T_3} \dots (4 - 25)$$

The net power can be determined as follow:

$$\dot{W}_{net} = \dot{W}_T - \dot{W}_C \quad \dots \quad (4-26)$$

The rate of heat added in combustion chamber can be calculated as follow:

$$\dot{Q}_{add} = \dot{m}_f \times C.V \dots (4-27)$$

From equations (4 - 26) and (4 - 27) we can determine the thermal efficiency for cycle as follow:

$$\eta_{th} = rac{\dot{W}_{net}}{\dot{Q}_{add}} \dots \dots \dots \dots \dots (4-28)$$

Also we can calculate the specific fuel consumption for the cycle as follow:

We can determine the maximum theoretical thermal efficiency or Carnot efficiency (η_{carnot}) as follow:

$$\eta_{carnot} = 1 - \frac{T_{min}}{T_{max}} = 1 - \frac{T_1}{T_3} \dots \dots \dots (4 - 30)$$

Carnot efficiency calculated to compare with actual thermal efficiency and justify it.

In addition, we can determine Novicov efficiency (η_{NOV}) as follow;

$$\eta_{Nov} = 1 - \sqrt{\frac{T_{min}}{T_{max}}} = 1 - \sqrt{\frac{T_1}{T_3}} \dots \dots \dots (4 - 31)$$

4.4. PRE CALCULATIONS

In this study we will assume the type of fuel used is LPG which contents from 60% Propane (C_3H_8) and 40% Butane (C_4H_{10}) by volume

Stoichiometric combustion equation of Propane:

 $C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2$

Stoichiometric combustion equation of Butane:

 $C_4H_{10} + 6.5(O_2 + 3.76N_2) \rightarrow 4CO_2 + 5H_2O + 24.44N_2$

Actually in most gas turbines the mixture of fuel and air is very weak mixture, so we will assume the Percentage of excess air = 300% theoretical air.

Actual combustion equation of Propane can be written as follow:

 $C_3H_8 + 4 \times 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 15O_2 + 75.2N_2$

Actual combustion equation of Butane also can be written as follow:

 $C_4H_{10} + 4 \times 6.5(O_2 + 3.76N_2) \rightarrow 4CO_2 + 5H_2O + 19.5O_2 + 97.74$

From the above equation for actual combustion we will determine the actual $\left(\frac{A}{F}\right)_{ratio}$.

Firstly calculate the number of moles of oxygen required:

 $= (0.6 \times 4 \times 5) + (0.4 \times 4 \times 6.5) = 22.4 \ kmol_{0_2}/kmol_f$

And then calculate the mass of air required for 1 kmol of fuel:

$$=\frac{22.4*32}{0.233}=3076.394\ kg_a/kmol_f$$

To calculate the mass of air required for 1 kg of fuel we must calculate the molecular weight of fuel by using equation (4 - 7):

$$= 0.6 \times 44 + 0.4 \times 58 = 49.6 \ kg/kmol$$

Thus, the actual mass of air required for 1 kg of fuel or actual $\left(\frac{A}{F}\right)_{ratio}$:

$$\left(\frac{A}{F}\right)_{ratio} = \frac{3076.394}{49.6} = 62.024 \ kg_a/kg_f$$

Actual number of moles of air (n_a) can be calculated as follow:

 $n_a = 4 \times \lfloor (0.6 \times 5 \times 4.76) + (0.4 \times 6.5 \times 4.76) \rfloor = 106.624 \, kmol_a$ Mole fraction of fuel can be determined by using equation (4 – 8):

$$y_f = \frac{1}{1 + 106.624} = 0.009292$$

Mole fraction of air can be determined by using equation (4 - 10):

$$y_a = 1 - 0.009292 = 0.990708$$

Mass fraction of fuel can be determined by using equation (4 - 9):

$$x_f = \frac{1}{1 + 62.024} = 0.01587$$

Mass fraction of air can be determined by using equation (4 - 11):

$$x_a = 1 - 0.01587 = 0.98413$$

Molecular weight of air can be calculated by using equation (4 - 7):

$$M_a = 32 \times 0.21 + 28 \times 0.79 = 28.84 \ kg/kmol$$

Gas constant for air

$$R_a = \frac{R_u}{M_a} = \frac{8.314}{28.84} = 0.2883 \, kJ/kg. \, K$$

In Joule-Brayton cycle the working fluid flowing through compressor (process $1 \rightarrow 2$) is air, and the working fluid flow through combustion chamber and turbine (process $2 \rightarrow 3$ and process $3 \rightarrow 4$) can be assume the products of combustion. So to calculate the specific heat for the working fluid flow through combustion chamber and turbine we must determine the gravimetric analysis for products as shown in table 4.3

product	$n_i\left(rac{kmol}{kmol_f} ight)$	$y_i\left(\frac{n_i}{\sum n_i}\right)$	M _i	$m_i = M_i n_i$	$x_i\left(\frac{m_i}{\sum m_i}\right)$
<i>CO</i> ₂	3.4	0.03124	44	149.6	0.048
H_2O	4.4	0.04043	18	79.2	0.025
02	16.8	0.15438	32	537.6	0.172
N_2	84.224	0.77395	28	2358.727	0.755
	$\sum n_i = 108.824$	1.0000		$\sum m_i = 3124.672$	1.000

 Table 4.3: Volumetric and gravimetric analysis for combustion products

4.5. SOLVING METHODOLOGY

We will use MATLAB software to perform the thermodynamic model calculation. For a simple Joule-Brayton cycle, value of initial temperature T_1 , pressure ratio r_p , is entropic efficiency for compressor η_c and is entropic efficiency for turbine η_T are given.

Calculate initial value for T_{2s} according to the following equation and assume ($\gamma = 1.4$)

Then calculate the value of logarithmic mean temperature for process $1 \rightarrow 2s$ (LMT_{1-2s}) by using equation (4 – 22) as follow:

$$LMT_{1-2s} = \frac{T_{2s} - T_1}{\ln \frac{T_{2s}}{T_1}} \quad \dots \dots \dots (4-33)$$

The value of LMT_{1-2s} will used to calculate the value of specific heat for each constituent of air according to the equation (4 - 4), and then substitute in equation (4 - 5) to calculate the value of C_{p_a} , then we will substitute the value of C_{p_a} in equation (4 - 24) to determine a new value of T_{2s} . This value will compared with the previous value, if the desired tolerance is not reached we will use the new value of T_{2s} to calculate LMT_{1-2s} , then to calculate C_{p_a} , finally to calculate new value of T_{2s} . These procedures will repeated by iterative scheme to achieve the desired tolerance for T_{2s} . After this we can calculate the value of T_2 according to equation (4 – 14).

Next step we will assume predict initial value of T_3 to calculate the initial value of LMT₂₋₃by using equation (4 – 22) as follow:

$$LMT_{2-3} = \frac{T_3 - T_2}{\ln \frac{T_3}{T_2}} \quad \dots \dots \dots \dots (4 - 34)$$

Then calculate the value of specific heat of combustion products (CO_2, H_2O, N_2, O_2) according to equation (4 - 4) depend on the value of LMT₂₋₃ and then substitute in equation (4 - 5) to calculate the value of $C_{p_{mix}}$, then we will conduct heat balance in combustion chamber to calculate the new value of T_3 according to the following equation:

$$\dot{m}_f \times C.V = (\dot{m}_a + \dot{m}_f) \times C_{p_{mix}} \times (T_3 - T_2) \qquad \dots \dots \dots (4 - 35)$$

This value will compared with the previous value, if the desired tolerance is not reached we will use the new value of T_3 to calculate LMT_{2-3} , then to calculate $C_{p_{mix}}$, finally to calculate new value of T_3 . These procedures will repeated by iterative scheme to achieve the desired tolerance for T_3 .

Next step we will calculate initial value for T_{4s} according to the following equation and assume ($\gamma = 1.4$)

$$T_{4s} = T_3 (1/r_p)^{\frac{\gamma-1}{\gamma}} \dots \dots (4-36)$$

Then calculate the value of LMT_{3-4s} for process $3 \rightarrow 4$ sby using equation (4 – 22) as follow:

$$LMT_{3-4} = \frac{T_{4S} - T_3}{\ln \frac{T_{4s}}{T_3}} \quad \dots \dots \dots (4-37)$$

Then calculate the value of specific heat of combustion products (CO_2, H_2O, N_2, O_2) according to equation (4 - 4) depend on the value of LMT_{3-4s} and then substitute in equation (4 - 5) to calculate the value of

 $C_{p_{mix}}$, then we will substitute the value of $C_{p_{mix}}$ in equation (4 – 25) to determine a new value of T_{4s} . This value will compared with the previous value, if the desired tolerance is not reached we will use the new value of T_{4s} to calculate LMT_{3-4s}, then to calculate $C_{p_{mix}}$, finally to calculate new value of T_{4s} . These procedures will repeated by iterative scheme to achieve the desired tolerance for T_{4s} . After this we can calculate the value of T_{4ac} cording to the equation (4 – 15).

Finally we will calculate Net power, actual thermal efficiency, specific fuel consumption, Carnot efficiency andNovicov efficiency according to the equations (4 - 26), (4 - 28), (4 - 29), (4 - 30) and (4 - 31).

4.6. PROGRAM FLOW CHART



