Chapter Four

Thermodynamic Modeling

4.1. INTRODUCTION

In this chapter we will address the thermodynamic model for Diesel 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 conductthe thermodynamic model calculations, and then we will present the results that will be obtained when we execute the program.

4.2. DIESEL ENGINE THERMODYNAMIC CYCLE MODEL

Thermodynamic cycle model for Diesel engine consist of four processes as shown in fig. 4.1 as follow.

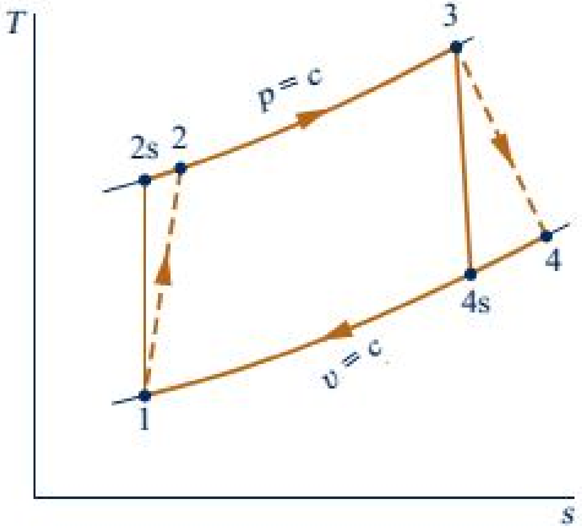


Fig. 4.1: T-s diagram of an air standard Diesel cycle model.

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 volume heat rejection process or an isochoric heat rejection process.

4.3. THERMODYNAMICMODEL 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:

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

Where:

C_p ≡The constant pressure specific heat (kJ/kg.K).

T ≡The temperature of air (K).

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

$$\boldsymbol{C_p - C_v = R} \qquad \dots\dots\dots \boldsymbol{(4-2)}$$

Where:

R ≡The gas constant of the air and equal [0.287] (kJ/kg.K).

The constant volume specific heat can be written as follow:

$$\left.\begin{array}{c} C_v = C_p - R = 2.506\times10^{-11}T^2 + 1.454\times10^{-7}T^{1.5} - 4.246\times10^{-7}T \\ +3.162\times10^{-5}T^{0.5} + 1.0433 - 1.512\times10^{4}T^{-1.5} + 3.063\times10^{5}T^{-2} \\ -2.212\times10^{7}T^{-3} \end{array}\right\} \ldots (4-3)$$

Where:

C_v ≡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 78.1% nitrogen, 20.95% oxygen, 0.92% 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 thegeneral form (reference [13]):

$$\frac{C_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \qquad \ldots\ldots\ldots (4-4)$$

Where:

R ≡The gas constant of the element (kJ/kg.K).

$a_1, a_2, \ldots a_5$ ≡ Constants.

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

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

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_2O	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(b): Coefficients for species temperature-dependent specific heats $[1000 < T < 3200\ K]$.

i	Species	a_1	a_2	a_3	a_4	a_5
1	CO_2	0.446080E+01	0.309817E-02	-0.123925E-05	0.227413E-09	-0.155259E-13
2	H_2O	0.271676E+01	0.294513E-02	-0.802243E-06	0.102266E-09	-0.484721E-14
3	N_2	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	0.362015E10	-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 76.51% nitrogen, 23.44% oxygen, and 0.05%carbon dioxide (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	**28.013**
2	O_2	**31.999**
3	CO_2	**44.010**

Thus, the specific heat at constant pressure for air can be obtained as follow:

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

Where:

C_{p_i} ≡ The specific heat at constant pressure for component ***i*** (kJ/kg.K).

x_i ≡ The mass fraction for component ***i***.

Also, the gas constant for air can be obtained as follow:

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

Where:

R_u ≡ The universal gas constant [8.3145] (kJ/kmol.K).

M_i ≡ The molecular weight for component ***i*** (kg/kmol).

Therefore, the specific heat at constant volume for air can be determined asfollow:

$$C_{v_{air}} = C_{p_{air}} - R_{air} \qquad \dots\dots\dots (4-7)$$

But for simplification, we will use the values of specific heat that given in equations (4 – 2) and (4 – 3).

After calculating the specific heats values,we can proceed to calculate the rate of heat added and heat rejected as follow:

$$\dot{Q}_{add} = \dot{m} \int_{T_2}^{T_3} C_p \, dT$$

$$= \dot{m} \left[\begin{array}{c} 8.353 \times 10^{-12} T^{3} + 5.816 \times 10^{-8} T^{2.5} - 2.123 \times 10^{-7} T^{2} \\ +2.108 \times 10^{-5} T^{1.5} + 1.3303 T + 3.024 \times 10^{4} T^{-0.5} - 3.063 \times 10^{5} T^{-1} \\ +1.106 \times 10^{7} T^{-2} \end{array} \right]_{T_2}^{T_3} \dots (4-8)$$

$$\dot{Q}_{rej} = \dot{m} \int_{T_1}^{T_4} C_v \, dT$$

$$= \dot{m} \left[\begin{array}{c} 8.353 \times 10^{-12} T^{3} + 5.816 \times 10^{-8} T^{2.5} - 2.123 \times 10^{-7} T^{2} \\ +2.108 \times 10^{-5} T^{1.5} + 1.0433 T + 3.024 \times 10^{4} T^{-0.5} - 3.063 \times 10^{5} T^{-1} \\ +1.106 \times 10^{7} T^{-2} \end{array} \right]_{T_2}^{T_3} \dots (4-9)$$

Where:

$\dot{m}$ ≡ The mass flow rate of working substance (kg/s).

For adiabatic compression (process 1 → 2) and adiabatic expansion(process 3 → 4), the compression and expansion efficiencies can be defined asfollow:

$$\boldsymbol{\eta_c = \frac{T_{2s} - T_1}{T_2 - T_1}} \qquad \dots\dots\dots (\mathbf{4-10})$$

$$\boldsymbol{\eta_e = \frac{T_3 - T_4}{T_3 - T_{4s}}} \qquad \dots\dots\dots (\mathbf{4-11})$$

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

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

$$\boldsymbol{TV^{\gamma-1} = (T + dT)(V + dV)^{\gamma-1}} \qquad \dots\dots\dots (\mathbf{4-12})$$

With Newton’s binomial of right side of equation (4 – 12) andbetake the small amounts, yields the fallowing relation:

$$\boldsymbol{(T + dT)(V + dV)^{\gamma-1} = (T + dT)(V^{\gamma-1} + (\gamma - 1)V^{\gamma-2}dV)} \quad \dots\dots\dots (\mathbf{4-13})$$

By rearranging the equation (4 – 12), we get:

$$(\gamma-1)\frac{dV}{V}=-\frac{dT}{T} \qquad \ldots\ldots\ldots(4-14)$$

By dividing the equation (4 – 7) on $C_{v_{air}}$ we get:

$$1=\gamma-\frac{R}{C_v} \qquad or \qquad (\gamma-1)=\frac{R}{C_v} \quad \ldots\ldots\ldots(4-15)$$

Substituting $(\gamma-1)$into equation (4 – 14) and rearrange it, yields fallowing relation:

$$R\frac{dV}{V}=-C_v\frac{dT}{T} \qquad \ldots\ldots\ldots(4-16)$$

By integrating the equation (4 – 16) between i and j we get:

$$\int_i^j R\frac{dV}{V}=\int_i^j -C_v\frac{dT}{T} \qquad \rightarrow \qquad R\ln\frac{V_i}{V_j}=C_v\ln\frac{T_j}{T_i} \quad \ldots\ldots\ldots(4-17)$$

Where the temperature in equation of C_v is:

$$T=\frac{T_j-T_i}{\ln\frac{T_j}{T_i}} \qquad \ldots\ldots\ldots(4-18)$$

The compression and cutoff and expansion ratios for diesel cycle are defined as follow:

Compression ratio: $r_v=\frac{V_1}{V_2}$ $\ldots\ldots\ldots(4-19)$

Cut-off ratio: $r_c=\frac{V_3}{V_2}=\frac{T_3}{T_2}$ $\ldots\ldots\ldots(4-20)$

Expansion ratio: $r_e=\frac{V_4}{V_3}$ $\ldots\ldots\ldots(4-21)$

Substituting $V_4=V_1$into equation (4 – 21) we get:

$$r_e=\frac{V_1}{V_3}=\frac{V_1}{V_2}\times\frac{V_2}{V_3}=\frac{V_1}{V_2}\Big/\frac{V_3}{V_2}=r_v/r_c \qquad \ldots\ldots\ldots(4-22)$$

We can reformulate the equation (4 – 17) for reversible compression process (1 → 2s) and reversible expansion process (3 → 4s) respectively as follow:

$$\boldsymbol{R}\ln \boldsymbol{r_v} = \boldsymbol{C_v}\ln\frac{\boldsymbol{T_{2s}}}{\boldsymbol{T_1}} \quad \dots\dots\dots(4-23)$$

$$-\boldsymbol{R}\ln(\boldsymbol{r_v}/\boldsymbol{r_c}) = \boldsymbol{C_v}\ln\frac{\boldsymbol{T_{4s}}}{\boldsymbol{T_3}} \quad \dots\dots\dots(4-24)$$

In ideal thermodynamic models there are no heat losses from the system to surrounding, but actually cycle operation there will be certain heat loss from system to the surroundings due to finite temperature differences between working fluid and cylinder wall. The amount of heat loss through the cylinder wall has been assumed to be proportional to the average temperature of heat addition and cylinder wall temperaturewhich is given as follow:

$$\dot{\boldsymbol{Q}}_{\boldsymbol{loss}} = \dot{\boldsymbol{m}}\boldsymbol{B}(\boldsymbol{T_2} + \boldsymbol{T_3} - 2\boldsymbol{T_0}) \quad \dots\dots\dots(4-25)$$

Where:

B ≡ Heat leakage coefficient of the cylinder wall (kJ/kg.K).

T_0 ≡The average temperature of the working fluid and cylinder walls (K).

Can be obtained$T_0$by calculating the logarithmic mean temperature between T_2 and T_3 as follow:

$$\boldsymbol{T_0} = \frac{\boldsymbol{T_3} - \boldsymbol{T_2}}{\ln\frac{\boldsymbol{T_3}}{\boldsymbol{T_2}}} \quad \dots\dots\dots(4-26)$$

There is another type of losses due to piston friction has been considered assuming a dissipation term which represented by friction force which is in linear function of mean piston velocity gives as follow:

$$\boldsymbol{f_\mu} = \boldsymbol{\mu v} = \boldsymbol{\mu}\frac{\boldsymbol{dx}}{\boldsymbol{dt}} \quad \dots\dots\dots(4-27)$$

Where:

μ ≡ Friction coefficient for global losses (N.s/m).

x ≡ Piston displacement (m).

Therefore, the power loss due to friction is given as follow:

$$\boldsymbol{P_\mu = \frac{dW_\mu}{dt} = \left(\mu \frac{dx}{dt}.dx\right)/dt = \mu v^2} \qquad \dots\dots\dots(\mathbf{4-28})$$

Where:

$v \equiv$ Mean piston speed (m/s).

Mean piston speed can be obtained for four stoke cycle engine as follow:

$$\boldsymbol{v = 4LN} \qquad \dots\dots\dots(\mathbf{4-29})$$

Where:

$L \equiv$ Stroke length of the cylinder (m).

$N \equiv$ The rotational speed of the engine (rev/sec).

Finally, the net power out and the thermal efficiency can be obtained by the following equations:

$$\boldsymbol{P_{net} = \dot{Q}_{add} - \dot{Q}_{rej} - P_\mu} \qquad \dots\dots\dots(\mathbf{4-30})$$

$$\boldsymbol{\eta_{th} = \frac{P_{net}}{\dot{Q}_{add} + \dot{Q}_{loss}}} \qquad \dots\dots\dots(\mathbf{4-31})$$

4.4. SOLVING METHODOLOGY

We will use MATLAB software to perform the thermodynamic model calculation. For a particular engine, value of initial temperature T_1, maximum temperature T_3, compression ratior_v,compression efficiency$\eta_c$and expansion efficiency $\eta_e$are given.

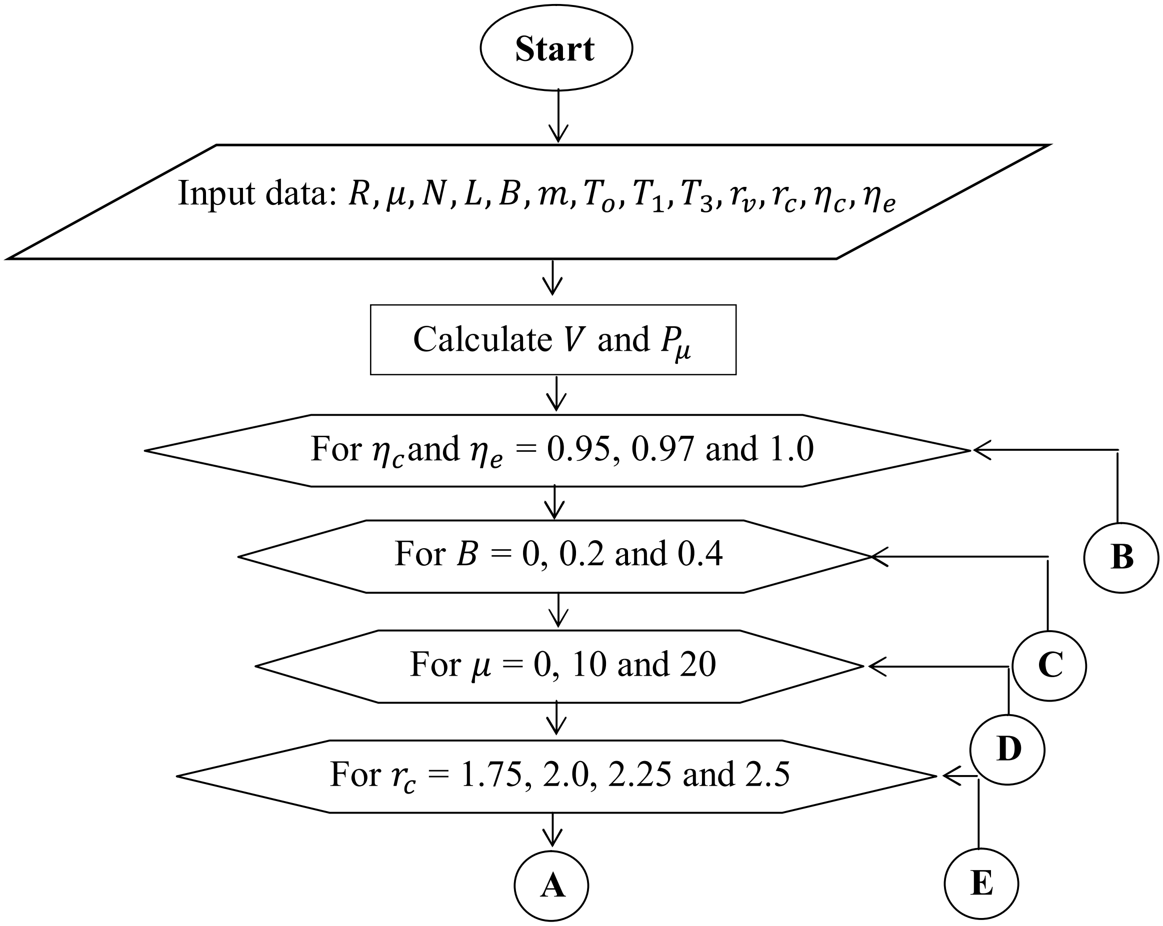
The first assumption for T_{2s} and T_{4s} can be obtained from the following equations by assuming an ideal cycle

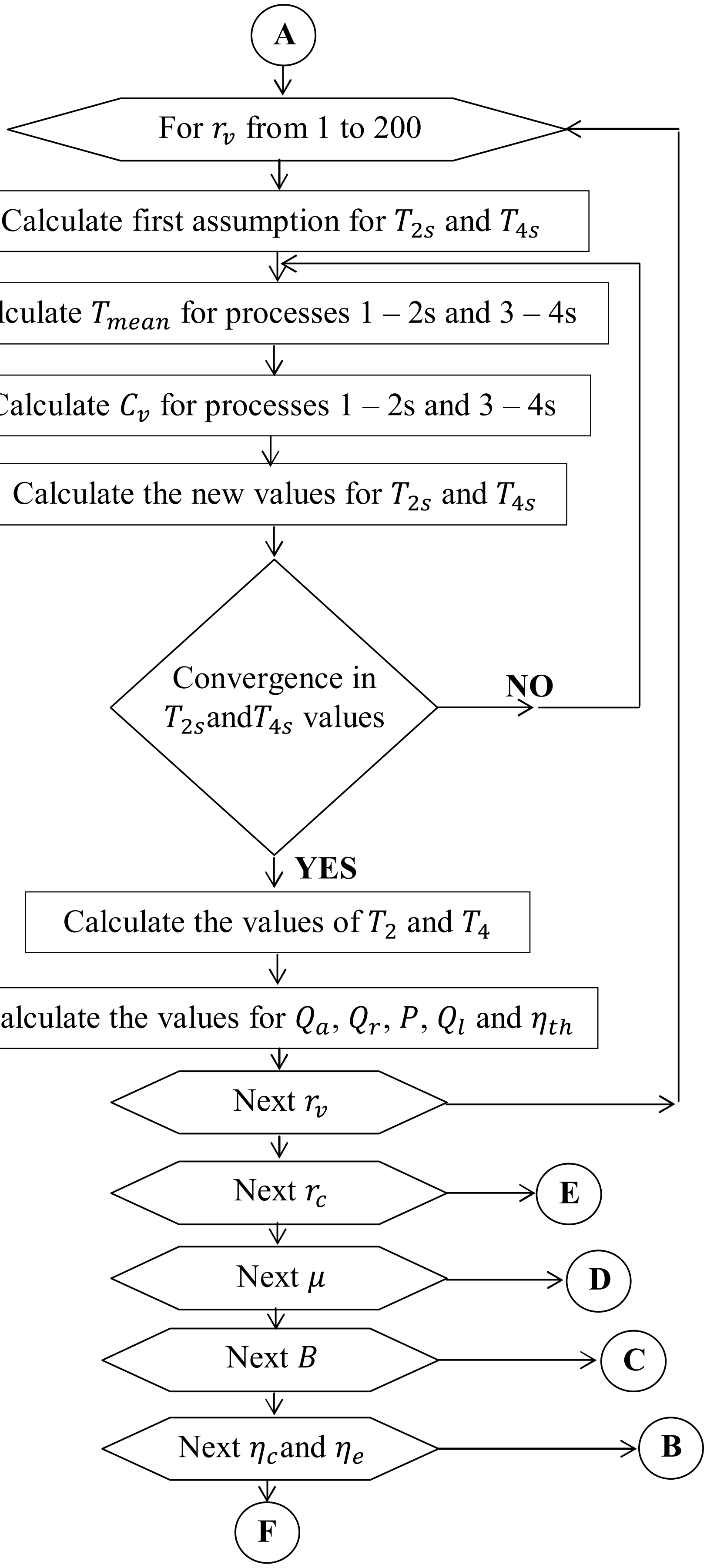
$$\boldsymbol{T_{2s} = T_1(r_v)^{\gamma-1}} \qquad \dots\dots\dots(\mathbf{4-32})$$

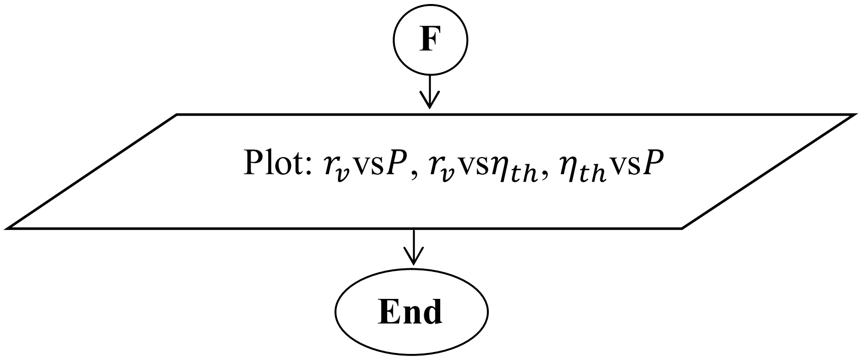
$$\boldsymbol{T_{4s} = T_3(r_c/r_v)^{\gamma-1}} \qquad \dots\dots\dots(\mathbf{4-33})$$

Assume the value of γ is equal 1.4, substituting the value of T_{2s}in first time and T_{4s}in second time in equation (4 – 18) to calculate the value of T which will be substituted in the equation of $C_v$to get it, after that substitute the value of C_v to get the new values of T_{2s} and T_{4s}, these new values are substituted in equations (4 – 2) and (4 – 3) to get the new value ofC_p andC_v respectively, this procedure will be repeated by iterative scheme until reach to the desired convergence. The values of T_2 and T_4 can be obtained from equations (4 – 10) and (4 – 11). Rate of heat transfer loss and friction loss are obtained from equation (4 – 25) and equation (4 – 27) respectively. Finally power output and efficiency of the cycle can be calculated using equation (4 – 30) and (4 – 31) respectively.

4.5. PROGRAM FLOW CHART




A
For r_v from 1 to 200
Calculate first assumption for T_{2s} and T_{4s}
Calculate T_{mean} for processes 1 – 2s and 3 – 4s
Calculate C_v for processes 1 – 2s and 3 – 4s
Calculate the new values for T_{2s} and T_{4s}
Convergence in T_{2s}andT_{4s} values
NO
YES
Calculate the values of T_2 and T_4
Calculate the values for Q_a, Q_r, P, Q_l and η_{th}
Next r_v
Next r_c
E
Next μ
D
Next B
C
Next $\eta_c$and η_e
B
F


F
Plot: r_v vs P, r_v vs η_{th}, η_{th} vs P
End