ME 146 Project 3: Hybrid Solar Gas Turbine - Design and Analysis

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Introduction

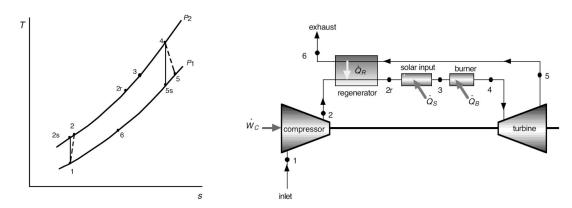


Fig. 1: T-S Diagram of Turbine System

Fig. 2: Schematic of Turbine System

The purpose of this project is to construct a computer simulation of the performance of the gas turbine system shown in Figure 1 and 2 above. Using MATLAB, we built our own codes to calculate the values of constants in Task 1, 2 and 3. Then, by utilizing our results from tasm 1, 2 and 3, it was possible to implement and answer the questions on task 4 and 5.

Combustor Governing Equations

In the combustor,

$$\begin{array}{l} \bullet \quad (\frac{\alpha}{4.76})(O_2 + 3,76N_2) + [\gamma C_3 H_8 + (1-\gamma)CH_4] \Rightarrow (\frac{3.76\alpha}{4.76})N_2 + (\frac{\alpha}{4.76} - 3\gamma - 2)O_2 + (2+2\gamma)H_2O \\ (\frac{3.76\alpha}{4.76})N_2 + (\frac{\alpha}{4.76} - 3\gamma - 2)O_2 + (2+2\gamma)H_2O + (1+2\gamma)CO_2 \end{array} \quad \text{[Eqn. 1]}$$

$$\bullet \quad \alpha = \alpha_{stoch} = 4.76(2 + 3\gamma)$$
 [Eqn. 2]

•
$$\sum_{reactants} \dot{\mathbf{n}}_r \hat{\mathbf{h}}_r = \sum_{products} \dot{\mathbf{n}}_p \hat{\mathbf{h}}_p$$
 [Eqn. 3]

•
$$(\frac{\alpha}{4.76})\hat{\mathbf{h}}_{O_2}[T_r] + (\frac{3.76\alpha}{4.76})\hat{\mathbf{h}}_{N_2}[T_r] + \gamma\hat{\mathbf{h}}_{C_3H_8}[T_r] + (1-\gamma)\hat{\mathbf{h}}_{CH_4}[T_r]$$

$$\left(\frac{\alpha}{4.76} - 3\gamma - 2\right)\hat{\mathbf{h}}_{O_2}[T_p] + (2 + 2\gamma)\hat{\mathbf{h}}_{H_2O}[T_p] + (1 + 2\gamma)\hat{\mathbf{h}}_{CO_2}[T_p]$$
 [Eqn. 4]

•
$$h_i(T) = h_i^{\circ}(T^{\circ}) + \hat{c}_{p,i}(T_{avg})(T - T^{\circ})$$
, where $T_{avg} = 0.5(T_r + T_p)$ [Eqn. 5]

•
$$\hat{\mathbf{h}}_{i}(T) = \hat{\mathbf{h}}_{i}^{\circ}(T^{\circ}) + \hat{\mathbf{c}}_{p,i}(T_{avg})(T - T^{\circ}), \text{ where } T_{avg} = 0.5(T_{r} + T_{p})$$
 [Eqn. 5]
• $\alpha = \frac{4.76[-\gamma \hat{\mathbf{h}}_{C_{3}H_{8}}[T_{r}] - (1-\gamma)\hat{\mathbf{h}}_{CH_{4}}[T_{r}] - (3\gamma+2)\hat{\mathbf{h}}_{O_{2}}[T_{p}] + (2+2\gamma)\hat{\mathbf{h}}_{H_{2}O}[T_{p}] + (1+2\gamma)\hat{\mathbf{h}}_{CO_{2}}[T_{p}]]}{[\hat{\mathbf{h}}_{O_{2}}[T_{r}] + 3.76\hat{\mathbf{h}}_{N_{2}}[T_{r}] - 3.76\hat{\mathbf{h}}_{N_{2}}[T_{p}] - \hat{\mathbf{h}}_{O_{2}}[T_{p}]]}$ [Eqn. 6]

•
$$\hat{c}_v = \hat{c}_p - \overline{R}$$
 (kJ/kmolK) [Eqn. 7]

•
$$\hat{\mathbf{c}}_{p,product} = y_{H_2O}\hat{\mathbf{c}}_{p,H_2O} + y_{CO_2}\hat{\mathbf{c}}_{p,CO_2} + y_{N_2}\hat{\mathbf{c}}_{p,N_2} + y_{O_2}\hat{\mathbf{c}}_{p,O_2}$$
 [Eqn. 8]
• $\hat{\mathbf{c}}_{v,prod} = \hat{\mathbf{c}}_{p,prod} - \overline{R}$ (kJ/kmolK) [Eqn. 9]

•
$$\hat{c}_{v,prod} = \hat{c}_{p,prod} - \overline{R}$$
 (kJ/kmolK) [Eqn. 9]

System Analysis Governing Equations

$$\epsilon_{regen} = \frac{\hat{n}\hat{c}_{p,air}(T_{2r}-T_{2})}{(\hat{n}\hat{c}_{p})_{min}(T_{5}-T_{2})}$$
 [Eqn.10]
$$\theta_{class} = \frac{\eta_{t} \cdot [1-(P_{1}/P_{2})^{(k-1)/k}] - (1/\eta_{c}) \cdot (T_{1}/T_{4}) \cdot [(P_{2}/P_{1})^{(k-1)/k} - 1]}{1-\epsilon_{r} \cdot [1-\eta_{t}+\eta_{t} \cdot [1-(P_{1}/P_{2})^{(k-1)/k}] - (1-\epsilon_{r}) \cdot (T_{1}/T_{4}) \cdot [1-(1/\eta_{c}) \cdot (P_{2}/P_{1})^{(k-1)/k} - 1]}$$
 [Eqn.11]

$$\eta_{class} = \frac{\eta_r [1 - (P_1/P_2)^{(k-1)/k}] - (1/\eta_c) \cdot (T_1/T_4) \cdot [(P_2/P_1)^{(k-1)/k} - 1]}{1 - \varepsilon_r \cdot [1 - \eta_r + \eta_r \cdot [1 - (P_r/P_2)^{(k-1)/k}] - (1 - \varepsilon_r) \cdot (T_r/T_r) \cdot [1 - (1/\eta_r) + (1/\eta_r) \cdot (P_2/P_r)^{(k-1)/k}]}$$
[Eqn 11]

•
$$n_{prod} = \alpha + \gamma + 1$$
 [Eqn 12]

•
$$m_{prod} = \overline{M_{N_2}} \frac{3.76\alpha}{4.76} + \overline{M_{O_2}} (\frac{\alpha}{4.76} - 3\gamma - 2) + \overline{M_{H_2O}} (2 + 2\gamma) + \overline{M_{CO_2}} (1 + 2\gamma)$$
 [Eqn 13]

$$\bullet \quad n_{air} = \frac{m_{air}}{\bar{M}_{air}}$$
 [Eqn 14]

•
$$n_{air}^{\cdot} = \frac{m_{air}}{M_{air}}$$
 [Eqn 14]
• $n_{prod}^{\cdot} = \frac{m_{air}}{M_{prod}^{\prime} n_{prod}}$ [Eqn 15]

$$\bullet \quad \eta_{system} = \frac{\dot{W}}{\dot{Q}} = \frac{W_t - \dot{W}_c}{\dot{Q}_b} = \frac{n_{products} \cdot c_{p,t} \cdot (T_4 - T_5) - \eta_{air} \cdot c_{p,c} \cdot (T_2 - T_1)}{n_{burner} \cdot c_{p,burner} \cdot (T_4 - T_3)}$$
[Eqn 16]

• Net Power:
$$\dot{P}_{out} = \dot{W}_{turbine, out} - \dot{W}_{req}$$
 [Eqn 17]

• Heat Input into Combustor:
$$\dot{Q}_{burner} = \dot{n}_{prod} \hat{c}_{p,prod} (T_4 - T_3)$$
 [Eqn 18]

• System efficiency:
$$\eta_{system} = \dot{P}_{out} / (\dot{Q}_{burner} + \dot{Q}_{solar})$$
 [Eqn 19]

Constants and Variables

- P_1 : Air at atmospheric pressure.
- T_1 : Inlet temperature
- T_2 : Compressor temperature.
- \overline{M} : The effective molecular mass
- m : Mass flow of air at the inlet.
- T_{af} : Adiabatic flame(exit) temperature
- T_r : Reactant temperature
- T_p : Product temperature
- a: Molar air-to-fuel ratio
 - (Moles of air) / (moles of propane and methane mixture) in inlet flow to burner
- γ : Fuel propane molar fraction
 - (Moles of Propane) / (moles of propane and methane in fuel mixture
- \hat{c}_{v} : Specific heat at constant volume.
- \hat{c}_p : Specific heat at constant pressure.
- \overline{R} : The universal gas constant.
- $\hat{c}_{v.prod}$: Average specific heat of product at constant volume.
- $\hat{c}_{p,prod}$: Average specific heat of product at constant pressure.
- ε_{regen} : Regenerator effectiveness.
- n : Molar flow
- h : enthalpy per kmol.
- \dot{Q}_{solar} : Solar heat input.

• η_{turb} : Turbine efficiency

• $\eta_{\textit{comp}}$: Compressor efficiency.

Responsibilities

This section provides a summary of how the project work was divided between the teammates when preparing this report.

Charles Lin:

- Introduction
- Task 4
- Task 5

Jung Hwan Ha:

- Task 1
- Task 2
- Task 3

Design Task Documentation

Task 1

Task Description:

The main objective of the task 1 is to build up our own computer program which has the ability to calculate the the molar air-to-fuel ration α that will occur in specified combustor adiabatic flame temperature(T_{af}) for given reactant temperature(T_r)

Assumptions/Idealizations:

- The values of α and γ are greater than or equal to the stoichiometric value.
- We assume $P_1 = 101 \text{ kPa}$.
- We assume $T_1 = 25$ °C which also can be $T_1 = 298.15$ K.
- We assume $\overline{M} = 28.97 \text{ kg/kmol}$.
- We assume $\dot{m} = 6.0 \text{ kg/s}$.
- We assume air as an ideal gas.
- We assume the stoichiometric mixture has enough oxygen to burn all propane and methane, and make them convert to oxygen and carbon dioxide.
- We assume the regenerator heated air and injected fuel to be at the same temperature.
- We assume water exists as water vapor in the exhaust gas.
- $\bullet \quad T_{avg} = 0.5(T_r + T_P).$
- T_{af} is greater than $T_{af, stoich}$.
- α is greater than α_{stoich} .
- $T^{\circ} = 25 \,^{\circ}\text{C}$.
- $\bullet \quad T_r = 550K.$
- $T_p = 1900K$.

Algorithm Summary of the Program:

- 1. After the air flows into the inlet, the mixture of propane(C_3H_8) and methane(C_3H_4) will be injected to the burner. And those will be completely burned.
- 2. Due to the combustion process of propane and methane, the chemical reaction of the combustion will be occured. And, the balanced chemical reaction can be written as [Eqn 1].
- 3. For stoichiometric conditions, the α can be determined as [Eqn 2].
- 4. Based on the [Eqn 3], [Eqn 4] can be derived in order to find the value of the molar air-to-fuel ratio α
- 5. Before calculating the enthalpy of each gas species, refer to the [Table 2] at [Appendix B], evaluate specific heat of each gas species.
- 6. After determining specific heat of each gas species, according to [Table 1] at [Appendix B], [Eqn 5] is used to determine each enthalpy of each gas species at reference temperature.

7. Rearranging [Eqn 1], it is possible to derive [Eqn 6] to solve for the air-to-ratio.

Required Deliverables for Given Conditions:

- 1. Value of α when the gas mixture is only composed with pure propane.
- 2. Value of α when the gas mixture is only composed with pure methane.
- 3. Value of α when the gas mixture is 50% mole fraction mixture.

Results:

Conditions of Gas Mixture	Value of α
Pure propane	39.5023
Pure methane	15.2750
50% mole fraction mixture	27.3887

Task 2

Task Description:

Build up our own computer program to compute the exit condition from the compressor and the work required per kilogram of air.

Assumptions/Idealizations:

- We assume $P_1 = 101 \text{ kPa}$.
- We assume $T_1 = 25$ °C which also can be $T_1 = 298.15$ K.
- We assume $\overline{M} = 28.97 \text{ kg/kmol}$.
- We assume $\dot{m} = 6.0 \text{ kg/s}$.
- We assume air as an ideal gas.
- $\bullet \quad T_{avg} = 0.5(T_r + T_P).$
- At $T_1 = 25$ °C, the molar enthalpy is zero.
- $P_2 = 130 \,\mathrm{Kpa}$.
- $\eta_{comp} = 1$

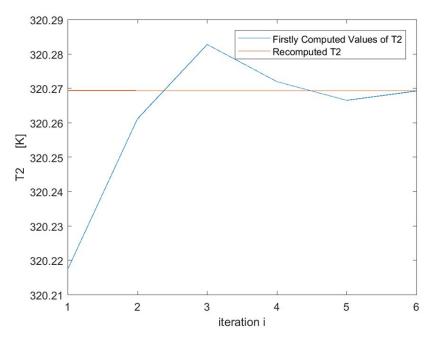
Algorithm summary of the program:

- 1. Guess the exit temperature, T_2 .
- 2. Compute specific heat of the product at the average temperature by using [Table 2] at [Appendix B].
- 3. Compute \hat{c}_{ν} by using [Eqn 7].

- 4. Using constant \hat{c}_p and \hat{c}_v , determine the enthalpy per kmol of air and the temperature at the ext from the compressor T_2 .
- 5. Recalculate the average temperature using the newly computed T_2 value and repeat the calculation of the outlet condition.
- 6. If the difference between T_2 and $T_{2, new}$ is less than 0.2, terminate the iterative calculation. If not, repeat the iteration from step 1-5 again.

Results:

Our resulting compressor temperature is 320.2694[K], shown in [Fig. 3]. The work required per kilogram of air is 134.3031[kW/kg of air]



[Fig. 3]: $T_2[K]$ over the Number of Iterations [i] at $P_2 = 130 \ kPa$ and $\eta_{comp} = 1$

Task 3

Task Description:

Task 3 is independent computer program which calculates $\hat{c}_{p,prod}$ for the gas mixture as the mole-fraction computed average of the \hat{c}_p values for the individual species(CO_2, O_2, H_2O, N_2) in the gas mixture that can be expressed as a function of molar-air-fuel ratio α .

Assumptions/Idealizations:

- We assume $P_1 = 101 \text{ kPa}$.
- We assume $T_1 = 25$ °C which also can be $T_1 = 298.15$ K.
- We assume $\overline{M} = 28.97 \text{ kg/kmol}$.

- We assume $\dot{m} = 6.0 \text{ kg/s}$.
- We assume air as an ideal gas.
- $\bullet \quad \gamma = 0.25$
- $T_p = 600K$

Algorithm Summary of the Program:

- 1. Calculate the total moles of product: which is equal to $n_{total} = \alpha + \gamma + 1$
- 2. Compute each molar fraction of each gas species in the gas mixture.
 - a. $y_{N_2} = \frac{3.76\alpha}{4.76n_{total}}$
 - b. $y_{O_2} = (\frac{\alpha}{4.76} 3\gamma 2) / n_{total}$ c. $y_{H_2O} = \frac{2+2\gamma}{n_{total}}$ d. $y_{CO_2} = \frac{1+2\gamma}{n_{total}}$

For the value of α , We use $\alpha_{stoich} = 4.76(2 + 3\gamma) = 4.76(2 + 3(0.25)) = 13.09$ due to the condition in Task 3.

- 3. Bring the calculated values of specific heats of each species in the gas mixture in Task 1.
- 4. Plug the result of step 2 and step 3 into the [Eqn 8], then it is possible to get the value of $\hat{c}_{p,prod}$ at temperature = 600K.
- 5. Refer to the [Table 2] at [Appendix B], compute \hat{c}_p for pure air at the same temperature.

Results:

At product gases at $T_p = 600K$, the following results are achieved from our own computer program.

$\hat{\mathbf{c}}_{p,prod}$ for stoichiometric combustion	33.0953 [kJ/kmol·k]
\hat{c}_p for pure air at $T_P = 600K$	30.5943[kJ/kmol·k]

Task 4

Task description:

In this task, we bring together our programs from Tasks 1, 2, and 3 to conduct overall system analysis. That is, given a P_1 , T_1 , P_2 , T_4 , γ , \dot{Q}_{solar} , η_{comp} , η_{turb} , and ε_{regen} , we may compute system net power output \dot{P}_{out} , heat input into the combustor \dot{Q}_{burner} , and system efficiency η_{system} . This system efficiency η_{system} is to be compared against η_{class} , an efficiency found by derivation in class from the constant specific heat relation.

Assumptions/Idealizations:

- We assume $P_1 = 101 \text{ kPa}$.
- We assume $T_1 = 25$ °C which also can be $T_1 = 298.15$ K.
- We assume $\overline{M} = 28.97 \text{ kg/kmol}$.
- We assume $\dot{m} = 6.0 \text{ kg/s}$.
- We assume air as an ideal gas.
- $T_{avg} = 0.5(T_r + T_P)$.
- At $T_1 = 25$ °C, the molar enthalpy is zero.
- $P_2 = 500 \,\text{kPa}$.
- $T_A = 1600 \text{ K}.$
- $\bullet \quad \eta_{comp} = 0.85$
- $\eta_{turb} = 0.85$
- $\dot{Q}_{solar} = 0$
- $\varepsilon_{regen} = 0.75$
- Initial α ratio is stoichiometric as given by [Eqn 2]

Algorithm summary of the program:

- 1. Initialize constants and assumptions
- 2. Initiate a for-loop with 2 iterations:
 - a. Call the Task2 program as a function to find the enthalpy, temperature, and work input required \dot{W}_{req} at State 2.
 - b. Guess $T_{5,guess}$. For the turbine expansion process, calculate $\widehat{c}_{p,prod}$. Use constant \widehat{c}_p and \widehat{c}_v analysis [Eqn 7] and [Eqn 9] in order to calculate T_5 . Implement bisection method to converge upon a T_5 value with error $\left|T_5 T_{5,guess}\right| < 0.2 \,^{\circ}\text{C}$.
 - c. For the regenerator, find the $\hat{c}_{p,air}$ and $\hat{c}_{p,prod}$ values at $T_{avg} = 0.5(T_2 + T_5)$. Solve for T_{2r} using [Eqn 10] and thermodynamic equations.
 - d. Find T_3 using an energy balance with \dot{Q}_{solar} . Because $\dot{Q}_{solar} = 0$, T_3 will be equal to T_{2r} ; the relevant $\hat{c}_{p,air}$ may also be found using Task 3 at T_{2r} .
 - e. Utilize the Task 1 program (implemented as "Task4supp") to find the corrected α value using T_4 and the T_3 we found. Go through steps (b) through (d) in the second iteration to recalculate the aforementioned values.
- 3. Upon completing the for-loop, solve for \dot{P}_{out} , \dot{Q}_{burner} , and η_{system} using Eqns. [Eqn 17], [Eqn 18], and [Eqn 19]. Compare η_{system} to η_{class} , which is found using [Eqn 11].
 - a. $\dot{P}_{out} = \dot{W}_{turbine, out} \dot{W}_{req}$
 - b. $\dot{Q}_{burner} = \dot{n}_{prod} \hat{c}_{p,prod} (T_4 T_3)$
 - c. $\eta_{system} = \dot{P}_{out}/(\dot{Q}_{burner} + \dot{Q}_{solar})$
 - d. η_{class}

Results:

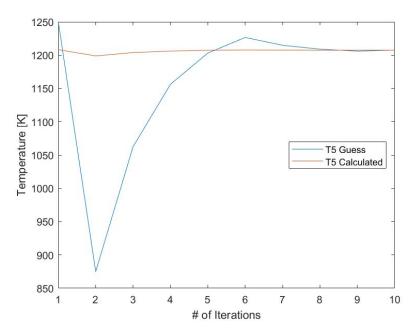


Fig. 4: Convergence of T_5

We see that in Figure 4 that our bisection method T_5 indeed converges. Our resulting deliverable values are as follows:

- $\dot{P}_{out} = 2070.3 \text{ kW}$
- $\dot{Q}_{burner} = 4735.0 \,\mathrm{kW}$
- $\bullet \quad \eta_{system} = 0.4372$
- $\bullet \quad \eta_{class} = 0.4284$

Additionally, we found the following intermediate or state values:

- $\alpha_{stoich} = 13.0900$
- $\alpha_{corrected} = 51.2669$
- $T_2 = 497.4372 \text{ K}$
- $T_3 = 1000.8 \,\mathrm{K}$
- $T_5 = 1207.5 \text{ K}$
- $\dot{W}_{turbine, out} = 3290.0 \,\mathrm{kW}$
- $\dot{W}_{reg} = 1219.7 \,\text{kW}$

Task 5(a) and (b)

Task description:

(a): Using the system analysis program created in Task 4, we are to take into account variation of \dot{Q}_{solar} during the day from 0 MW (nighttime) to 2.0, 2.5, and 3.0 MW. We are to determine the resulting

changes in net power output \dot{P}_{out} , heat input into the combustor \dot{Q}_{burner} , and system efficiency η_{system} compared to η_{class} .

(b): Using the system analysis program created in Task 4, we are to take into account variation of the mole fraction of propane γ within a range of 0 to 0.5 and understand the impact upon system performance.

Assumptions/Idealizations:

All assumptions from Task 4 hold, with the following changes for parts (a) and (b):

- (a) $\dot{Q}_{solar} = 0, 2.0, 2.5, 3.0 \,\text{MW}, \, \gamma = 0.25$
- (b) Assume $\dot{Q}_{solar} = 0$, $\gamma = 0$, 0.25, 0.5

Algorithm summary of the program:

The algorithm summary is identical to that of Task 4, with one exception - because \dot{Q}_{solar} changes, T_3 is no longer equal to T_{2r} . As a result, T_3 must also be guessed and solved using the bisection method as with finding T_5 .

Results:

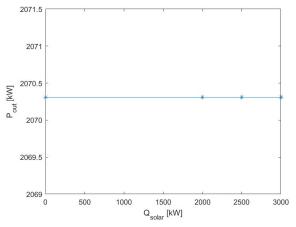
(a)

\dot{Q}_{solar} [kW]	\dot{Q}_{burner} [kW]	$\dot{P}_{out}[kW]$	η_{system}	$\eta_{\it class}$
0	4734.633591	2070.308434	0.4372689869	0.4283605165
2000	2432.743426	2070.308434	0.4670490112	0.4283605165
2500	1882.982015	2070.308434	0.4723515695	0.4283605165
3000	1341.885428	2070.308434	0.4768224469	0.4283605165

Table 1

Our deliverables are tabulated in Table 1 above. \dot{P}_{out} stays constant throughout variation in \dot{Q}_{solar} . As seen in Eqn. [17], \dot{P}_{out} is only dependent upon $\dot{W}_{turbine,\,out}$ and \dot{W}_{req} . As $\dot{W}_{turbine,\,out}$ is primarily dependent on the difference between the constant T_4 and T_5 (which also turns out to be constant across varying \dot{Q}_{solar} values), $\dot{W}_{turbine,\,out}$ is constant throughout the day. Additionally, \dot{W}_{req} is dependent upon the assumed constants P_2 and η_{comp} , and is therefore itself constant. Thus, it makes sense for \dot{P}_{out} to be constant throughout the day, as seen in Figure 5.

However, system efficiency actually increases as \dot{Q}_{solar} increases (Figure 6). We also note that the required heat input into the combustor \dot{Q}_{burner} decreases as \dot{Q}_{solar} increases (Figure 7). As efficiency is the net power output over the total heat input, we see that the increases in system efficiency is due to the decrease in required \dot{Q}_{burner} , not because of an increase in \dot{P}_{out} .



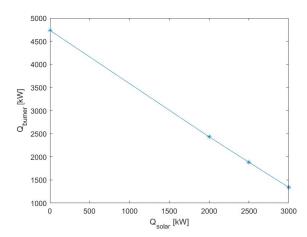


Fig. 5: \dot{P}_{out} over \dot{Q}_{solar}

Fig. 6: \dot{Q}_{burner} over \dot{Q}_{solar}

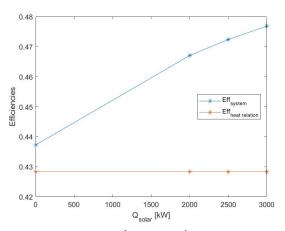


Fig. 7: \dot{P}_{out} over \dot{Q}_{solar}

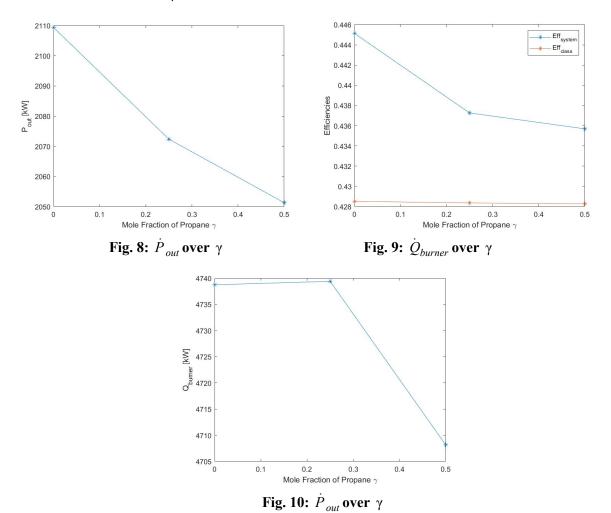
(b)

Propane Mole Fraction Ratio				
γ	\dot{Q}_{burner} [kW]	$\dot{P}_{out}[\mathrm{kW}]$	η_{system}	η_{class}
0	4738.746897	2109.342238	0.4451265881	0.4285166515
0.25	4739.410797	2072.368703	0.4372629409	0.4283605165
0.5	4708.183244	2051.3234	0.435693195	0.4282737671

Table 2

System performance across variation of the propane mole fraction ratio γ is tabulated above in Table 2.

As Figure 8 demonstrates, as γ increases, \dot{P}_{out} decreases. Meanwhile, as γ increases, the required heat input \dot{Q}_{burner} decreases. However, this decrease is not enough to maintain system efficiency η_{system} levels, and it thus decreases over γ .



Appendix A: MATLAB Code

Task1.m

```
%% Task 1 Problem Statement
% Find molar air-to-fuel ratio alpha for i) pure propane, ii) pure
methane,
    iii) 50% mixture
%% Initializing Constants/Assumptions
Tr = 550; %[K]
Tp = 1900; %[K]
Tavg = (Tr + Tp)/2;
To = 25+273; %[K] from 25 oC
% Fuel Propane ratios for i) pure propane, ii) pure methane,
% iii) 50 percent mixture
q1 = 1;
g2 = 0;
g3 = 0.5;
%% Finding h i(T) Molar Enthalpy for Gas Species i
% cp = a + bT + cT^2 + dT^3, for T = Tavg
% 6 Gas species:
   1) C3H8
    2) CH4
응
  3) 02
응
  4) H2O
   5) CO2
응
    6) N2
a = [-4.04 \ 19.89 \ 25.48 \ 32.24 \ 22.26 \ 28.90];
b = [30.48 \ 5.024 \ 1.520 \ 0.1923 \ 5.981 \ -0.1571].*10^-2;
c = [-15.72 \ 1.269 \ -0.7155 \ 1.055 \ -3.501 \ 0.8081].*10^-5;
d = [31.74 - 11.01 1.312 - 3.595 7.469 - 2.873].*10^-9;
cp=zeros(1,6);
for i=1:length(cp)
    cp(i) = a(i) + b(i)*Tavg + c(i)*Tavg^2 + d(i)*Tavg^3; %[kJ/(kmol*K)]
end
ho = [-103850 - 74850 \ 0 \ -241820 \ -393520 \ 0]; \ \%[kJ/kmol]
h = Q(n,T) ho(n) + cp(n)*(T-To); %Molar Enthalpy
```

Task2.m

```
%% Task 2 Problem Statement
% Compute exit condition from compressor and work required per kg of air
function [h2 out, T2 out, W req] = Task2(P2, eff comp)
    %% Initialize Constants/Assumptions
     P2 = 130;
     eff comp = 1;
   T1 = 298;
    P1 = 101; %[kPa]
    R = 8.314; %[kJ/(kmol*K)]
    h1 = 0; %enthalpy of air = 0 at 25oC
    mdot = 6.0; %[kg/s]
    M molar = 28.97; %[kg/kmol]
    %% Iteration
    error = [1000 1000 1000]; %Initialize error
    T2 = [298 \ 0 \ 1200]; %Initial guess range of <math>T2
    tol = 0.2; %Tolerance of 0.2 oC
    i=1;
    while abs(error(2))>tol %|| (error(1)*error(3)<0)
        mid(i) = (T2(1)+T2(3))/2;
```

```
T2(2) = mid(i);
        Tavg1 = (T1+T2)./2;
        %(ii-iv): Compute T2 calc1
        cp1 = 28.11 + Tavg1.*0.1967e-2 + Tavg1.^2.*0.4802e-5 +
Tavg1.^3.*-1.966e-9;
        cv1 = cp1-R;
        k1 = cp1./cv1; %Array
        T2s 1 = T1*(P2/P1).^((k1-1)./k1);
        T2 calc1 = T1 + (T2s 1-T1)./eff comp; %array
        %(v-vii): Compute T2 calc2, Recomputation using T2_calc1 for Tavg
        Tavg2 = (T1+T2 calc1)./2; %Array
        %(ii-iv): Compute T2 calc1
        cp2 = 28.11 + Tavg2.*0.1967e-2 + Tavg2.^2.*0.4802e-5 +
Tavg2.^3.*-1.966e-9;
        cv2 = cp2-R;
        k2 = cp2./cv2; %Array
        T2s 2 = T1*(P2/P1).^((k2-1)./k2);
        T2 calc2 = T1 + (T2s 2-T1)./eff comp;
        %Error for Higher and Lower Bounds
        error = T2 calc2-T2 calc1; %array
        if error(1)*error(2)<0
             T2(3) = T2(2);
        else
            T2(1) = T2(2);
        end
        %For plotting/debugging
        T2 \text{ result1(i)} = T2 \text{ calc1(2)};
        T2 \text{ result2(i)} = T2 \text{ calc2(2)};
        errorPlot(i) = error(2);
        cp result = cp2(2);
        i=i+1;
    end
    T2 \text{ out} = T2 \text{ result2 (end)};
    h2 \text{ out} = cp \text{ result*}(T2 \text{ out-T1}) + h1; %[kJ/kmol]
    W req = mdot*cp result/M molar*(T2 out-T1); %[kW]
    % Plots
      plot(T2 result1); hold on; plot(T2 result2);
```

```
% xlabel("Iterations i");
% ylabel("Temperature [K]");
end
```

Task3.m

```
%% Task 3 Problem Statement
% Compute cp prod for product gas mixture as mole-fraction weighed average
% of the cp values. Assume stoichiometric conditions.
function cp prod = Task3(a)
    %% Initializing Constants/Assumptions
    g = 0.25;
    Tavg = 600; %[K]
    % Test Case:
    % a stoich = 4.76*(2+3*g);
    % a = a stoich;
    mol\ total = (3.76*a/4.76) + (a/4.76 - 3*g - 2) + (2 + 2*g) + (1 + 2*g)
2*q);
    %% Molar Relations
    y N2 = [3.76*a/4.76] / mol total;
    y 02 = [a/4.76 - 3*g - 2] / mol total;
    y H20 = [2 + 2*g] / mol total;
    y CO2 = [1 + 2*g] / mol total;
       1) 02
      2) H2O
       3) CO2
      4) N2
    a = [25.48 \ 32.24 \ 22.26 \ 28.90];
    b = [1.520 \ 0.1923 \ 5.981 \ -0.1571].*10^-2;
    c = [-0.7155 \ 1.055 \ -3.501 \ 0.8081].*10^-5;
    d = [1.312 -3.595 7.469 -2.873].*10^-9;
    cp O2 = a(1) + b(1)*Tavg + c(1)*Tavg^2 + d(1)*Tavg^3; %[kJ/(kmol*K)]
    cp_{H20} = a(2) + b(2)*Tavg + c(2)*Tavg^2 + d(2)*Tavg^3;
    cp CO2 = a(3) + b(3)*Tavg + c(3)*Tavg^2 + d(3)*Tavg^3;
```

Task4.m

```
%% Task 4 Problem Statement
%% Constants/Assumptions
mdot air = 6.0;
M = 28.97;
P1 = 101; %[kPa]
T1 = 298; %[K], 250C
P2 = 500; %[kPa]
T4 = 1600; %[K]
q = 0.25;
Qs = 0;
eff comp = 0.85;
eff turb = 0.85;
e regen = 0.75;
h1 = 0; %[kJ/kmol] - find enthalpies at other states by determining change
in enthalpy
R = 8.314; %[kJ/(kmol*K)]
a stoich = 4.76*(2+3*g);
a = a_stoich;
for z = 1:2
```

```
%% (i) Compressor
[h2, T2, W req] = Task2(P2, eff comp);
%% (ii)
% Implement Task3 where necessary
%% (iii & iv): Turbine Expansion Process
error = [1000 \ 1000 \ 1000];
T5 \text{ guess} = [500 \ 0 \ 2000];
tol = 0.2;
i=1;
while(abs(error(2))>tol)
    mid = (T5 guess(1) + T5_guess(3))/2;
    T5 guess(2) = mid;
    Tavg = 0.5*(T4+T5 \text{ guess});
    cp prod turbine = Task3(a,g,Tavg);
    cv prod turbine = cp prod turbine - R;
    k = cp prod turbine./cv prod turbine;
    T5 s = T4*(P1/P2).^{(k-1)./k};
    T5 calc = eff turb.*(T5_s - T4) + T4;
    error = T5 calc - T5 guess;
    %Tighten the T5 guess bounds
    if error(1)*error(2)<0
        T5 guess(3) = T5 guess(2);
    else
        T5 guess(1) = T5 guess(2);
    end
    T5 result(i) = T5 guess(2);
    T5 constant(i) = T5 calc(2);
    cp prod turbine result(i) = cp prod turbine(2);
    i=i+1;
end
T5 = T5 \text{ result(end)};
cp prod turbine out = cp prod turbine result(end);
%% (v): Regenerator
Tavg regen = 0.5*(T2 + T5 result(end));
[cp air regen, cp prod regen] = Task3(a,g,Tavg regen);
```

```
M N2 = 28.01;
    M 02 = 32.00;
    M H20 = 18.02;
    M CO2 = 44.01;
    n prod = 3.76/4.76*a + (a/4.76-3*g-2) + (2+2*g) + (1+2*g);
    m \text{ prod} = M N2*3.76/4.76*a + M O2*(a/4.76-3*g-2) + M H2O*(2+2*g) + ...
        M CO2*(1+2*g);
    ndot prod = mdot air/(m prod/n prod); % [kmol/s]
    ndot air = mdot air/M air; % [kmol/s]
    n cp air = ndot air*cp air regen;
    n cp prod = ndot prod*cp prod regen;
    n cp min = min([n cp air n cp prod]);
    syms T2 r
    eqn1 = e_regen == (n_cp_air)*(T2_r - T2)/(n_cp_min*(T5-T2));
    T2 r ans = double(solve(eqn1)); % [K]
    %% (vi): Find T3
    [f, cp air] = Task3(a,g,T2 r ans);
    T3 = Qs/(ndot_air*cp_air) + T2 r ans;
    % can only evaluate cp air at T2 r ans if T2 r ans = T3;
    % this is the case for Task 4; however, for Task 5, T2 r ans != T3;
    % For Task 5, cp air must be evaluated at Tavg of T2 r and T3.
    %% (vii) Compute a
    % Eq. 3
    a corrected = Task4supp(g, T3, T4);
    a result(z) = a corrected;
end
a result = a result(1);
%% Performance Calculations
W out = ndot prod*cp prod turbine out*(T4-T5);
%Tavg burner = 0.5*(T4-T3);
Tavg burner = T4;
cp prod burner = Task3(a result,g,Tavg burner);
Qburner = ndot prod*cp prod burner*(T4-T3); %Q for combustor
power out = W out-W req; %[W]
```

Task4supp.m

```
%% Task 4 Support: Implementing Task 1 as function
% Find molar air-to-fuel ratio alpha for i) pure propane, ii) pure
methane,
    iii) 50% mixture
%% Initializing Constants/Assumptions
function [a out] = Task4supp(g, Tr, Tp)
    % Tr = 550; %[K]
    % Tp = 1900; %[K]
    Tavg = (Tr + Tp)/2;
    To = 25+273; %[K] from 25 oC
    %% Finding h i(T) Molar Enthalpy for Gas Species i
    % cp = a + bT + cT^2 + dT^3, for T = Tavg
    % 6 Gas species:
      1) C3H8
       2) CH4
       3) 02
      4) H2O
       5) CO2
       6) N2
```

```
a = [-4.04 \ 19.89 \ 25.48 \ 32.24 \ 22.26 \ 28.90];
    b = [30.48 \ 5.024 \ 1.520 \ 0.1923 \ 5.981 \ -0.1571].*10^-2;
    c = [-15.72 \ 1.269 \ -0.7155 \ 1.055 \ -3.501 \ 0.8081].*10^-5;
    d = [31.74 - 11.01 1.312 - 3.595 7.469 - 2.873].*10^-9;
    cp=zeros(1,6);
    for i=1:length(cp)
        cp(i) = a(i) + b(i) *Tavg + c(i) *Tavg^2 + d(i) *Tavg^3;
%[kJ/(kmol*K)]
    end
    ho = [-103850 - 74850 \ 0 - 241820 - 393520 \ 0]; \ %[kJ/kmol]
    h = Q(n,T) ho(n) + cp(n)*(T-To); %Molar Enthalpy
    %% Finding alpha i for Cases (i), (ii), (iii)
    a out = 4.76*(-g*h(1,Tr) - (1-g)*h(2,Tr) - (3*g+2)*h(3,Tp) + ...
        (2+2*g)*h(4,Tp) + (1+2*g)*h(5,Tp)) / ...
        (h(3,Tr) + 3.76*h(6,Tr) - 3.76*h(6,Tp) - h(3,Tp));
end
```

Task5 ab.m

%% Constants/Assumptions

```
mdot_air = 6.0;
M_air = 28.97;
P1 = 101; %[kPa]
T1 = 298; %[K], 25oC
P2 = 500; %[kPa]
T4 = 1600; %[K]
g = 0.5;
Qs = 0;
eff_comp = 0.85;
eff_turb = 0.85;
e_regen = 0.75;
h1 = 0; %[kJ/kmol] - find enthalpies at other states by determining change in enthalpy
R = 8.314; %[kJ/(kmol*K)]
```

```
a stoich = 4.76*(2+3*g);
a = a stoich;
for z = 1:2
    %% (i) Compressor
    [h2, T2, W req] = Task2(P2, eff comp);
    %% (ii)
    % Implement Task3 where necessary
    %% (iii & iv): Turbine Expansion Process
    error = [1000 \ 1000 \ 1000];
    T5 guess = [500 \ 0 \ 2000];
    tol = 0.2;
    i=1;
    while(abs(error(2))>tol)
        mid = (T5 guess(1) + T5 guess(3))/2;
        T5 guess(2) = mid;
        Tavg = 0.5*(T4+T5 \text{ guess});
        cp prod turbine = Task3(a,g,Tavg);
        cv prod turbine = cp prod turbine - R;
        k = cp prod turbine./cv prod turbine;
        T5 s = T4*(P1/P2).^{(k-1)./k};
        T5_{calc} = eff_{turb.*}(T5 s - T4) + T4;
        error = T5 calc - T5 guess;
        %Tighten the T5 guess bounds
        if error(1)*error(2)<0</pre>
            T5 guess(3) = T5 guess(2);
        else
            T5 guess(1) = T5 guess(2);
        end
        T5 result(i) = T5 guess(2);
        T5 constant(i) = T5 calc(2);
        cp prod turbine result(i) = cp prod turbine(2);
        i=i+1;
    end
    T5 = T5 \text{ result(end)};
    cp prod turbine out = cp prod turbine result(end);
```

```
%% (v): Regenerator
Tavg regen = 0.5*(T2 + T5 result(end));
[cp air regen, cp prod regen] = Task3(a,g,Tavg regen);
M N2 = 28.01;
M 02 = 32.00;
M H20 = 18.02;
M CO2 = 44.01;
n prod = 3.76/4.76*a + (a/4.76-3*g-2) + (2+2*g) + (1+2*g);
m \text{ prod} = M \text{ N2*3.76/4.76*a} + M \text{ O2*(a/4.76-3*g-2)} + M \text{ H2O*(2+2*g)} + \dots
    M CO2*(1+2*g);
ndot prod = mdot air/(m prod/n prod); % [kmol/s]
ndot air = mdot air/M air; % [kmol/s]
n cp air = ndot air*cp air regen;
n cp prod = ndot prod*cp prod regen;
n cp min = min([n cp air n cp prod]);
syms T2 r
eqn1 = e regen == (n cp air)*(T2 r - T2)/(n cp min*(T5-T2));
T2 r ans = double(solve(eqn1)); % [K]
%% (vi): Find T3 iteratively - use cp air
    error3 = [1000 1000 1000];
    T3 guess = [400 \ 0 \ 1600];
    j=1;
    while(abs(error3(2))>tol)
        mid = (T3 guess(1) + T3 guess(3))/2;
        T3 guess(2) = mid;
        Tavg = 0.5*(T2 \text{ r ans}+T3 \text{ guess}); %array
        [cp prod, cp air] = Task3(a,g,Tavg); %arrays
        T3 calc = Qs./(ndot air.*cp air) + T2 r ans;
        error3 = T3 calc - T3 guess;
        %Tighten the T3 guess bounds
        if error3(1)*error3(2)<0
             T3 \text{ guess}(3) = T3 \text{ guess}(2);
        else
             T3 \text{ guess}(1) = T3 \text{ guess}(2);
```

```
end
            error out = error3(2);
            T3 result(j) = T3 guess(2); % Require resetting from
            T3 constant(j) = T3 calc(2);
            cp prod result(j) = cp prod(2);
            j = j + 1;
        end
        T3 = T3 \text{ result(end)};
        cp prod out = cp prod result(end);
    %% (vii) Compute a
    % Eq. 3
    a corrected = Task4supp(g, T3, T4);
    a result(z) = a corrected;
end
a result = a result(1);
%% Performance Calculations
W out = ndot prod*cp prod turbine out*(T4-T5);
%Tavg burner = 0.5*(T4-T3);
Tavg burner = T4;
cp prod burner = Task3(a result, g, Tavg burner);
Qburner = ndot prod*cp prod burner*(T4-T3); %Q for combustor
power out = W out-W req; %[W]
eff sys = power out/(Qs + Qburner);
eff class = (eff turb*(1-(P1/P2)^((k-1)/k)) -
(1/eff comp*T1/T4*((P2/P1)^((k-1)/k)-1)))/...
    (1-e regen*(1-eff turb+eff turb*(P1/P2)^((k-1)/k)) - ...
     (1-e regen)*(T1/T4)*(1-(1/eff comp) +
(1/eff comp) * (P2/P1) ^ ((k-1)/k)));
%% Results and Plot
% % Part (a)
% % resultsAdd = [Qs; Qburner; power out; eff sys; eff class];
% % Part (b)
% resultsAdd = [g; Qburner; power out; eff sys; eff class];
% results = [results resultsAdd];
%% Part (a)
% results =
```

```
[0,2000,2500,3000;4734.63359107193,2432.74342603970,1882.98201537437,1341.
88542803099;2070.30843392204,2070.30843392204,2070.30843392204,2070.308433
92204; 0.437268986944631, 0.467049011174485, 0.472351569470268, 0.476822446892
826; 0.428360516508602, 0.428360516508602, 0.428360516508602, 0.42836051650860
21;
% % Row 1: Qs Values
% % Row 2: Qburner
% % Row 3: Power Out
% % Row 4: System Efficiency
% % Row 5: Efficiency from Class Relation
% Qs vec = results(1,:);
% % Plot of Qburner over Varying Qs
% plot(Qs vec, results(2,:),'*-');
% xlabel("Q {solar} [kW]");
% ylabel("Q {burner} [kW]");
% % Plot of Net Power Out over Varying Qs
% figure;
% plot(Qs vec, results(3,:),'*-');
% xlabel("Q {solar} [kW]");
% ylabel("P {out} [kW]");
% % Plot of Efficiencies
% figure;
% plot(Qs vec, results(4,:),'*-'); hold on;
% plot(Qs vec, results(5,:),'*-');
% xlabel("Q {solar} [kW]");
% ylabel("Efficiencies");
% legend("Eff {system}","Eff {class}","Location","east");
%% Part (b)
% results =
[0,0.2500000000000,0.5000000000000;4738.74689668427,4739.41079682154,4
708.18324435581;2109.34223807536,2072.36870310773,2051.32340021501;0.44512
6588117901,0.437262940890787,0.435693194965200;0.428516651524242,0.4283605
16508602,0.428273767100242];
% % Row 1: q Values
% % Row 2: Qburner
% % Row 3: Power Out
% % Row 4: System Efficiency
% % Row 5: Efficiency from Class Relation
% g vec = results(1,:);
```

```
% % Plot of Qburner over Varying Qs
% plot(g vec, results(2,:),'*-');
% xlabel("Mole Fraction of Propane \gamma");
% ylabel("Q {burner} [kW]");
\mbox{\%} % Plot of Net Power Out over Varying Qs
% figure;
% plot(g vec, results(3,:),'*-');
% xlabel("Mole Fraction of Propane \gamma");
% ylabel("P {out} [kW]");
% % Plot of Efficiencies
% figure;
% plot(g vec, results(4,:),'*-'); hold on;
% plot(g vec, results(5,:),'*-');
% xlabel("Mole Fraction of Propane \gamma");
% ylabel("Efficiencies");
% legend("Eff {system}","Eff {class}","Location","northeast");
```

Appendix B: Thermodynamic Tables

Table A-25 Thermochemical Properties of Selected Substances at 298K and 1 atm

		Molar Mass, M (kg/kmol)	Enthalpy of Formation, \bar{h}_{r}^{o} (kJ/kmol)	Gibbs Function of Formation, \vec{g}_{1}^{o} (kJ/kmol)	Absolute Entropy, \$\overline{s}^{\circ}\$ (kJ/kmol · K)	Heating Values	
Substance	Formula					Higher, HHV (kJ/kg)	Lower, LHV (kJ/kg)
Carbon	C(s)	12.01	0	0	5.74	32,770	32,770
Hydrogen	H ₂ (g)	2.016	0	0	130.57	141,780	119,950
Nitrogen	N2(g)	28.01	0	0	191.50	-	_
Oxygen	O2(g)	32.00	0	0 .	205.03	_	
Carbon monoxide	CO(g)	28.01	-110,530	-137,150	197.54	_	_
Carbon dioxide	CO ₂ (g)	44.01	-393,520	-394,380	213.69	-	_
Water	H ₂ O(g)	18.02	-241,820	-228,590	188.72	_	_
Water	H ₂ O(l)	18.02	-285,830	-237,180	69.95	_	-
Hydrogen peroxide	H ₂ O ₂ (g)	34.02	-136,310	-105,600	232.63	-	
Ammonia	NH ₃ (g)	17.03	-46,190	-16,590	192.33		
Oxygen	O(g)	16.00	249,170	231,770	160.95	-	
Hydrogen	H(g)	1.008	218,000	203,290	114.61	_	-
Nitrogen	N(g)	14.01	472,680	455,510	153.19	_	_
Hydroxyl	OH(g)	17.01	39,460	34,280	183.75	_	-
Methane	CH ₄ (g)	16.04	-74,850	-50,790	186.16	55,510	50,020
Acetylene	C2H2(g)	26.04	226,730	209,170	200.85	49,910	48,220
Ethylene	C2H4(g)	28.05	52,280	68,120	219.83	50,300	47,160
Ethane	C₂H ₆ (g)	30.07	-84,680	-32,890	229.49	51,870	47,480
Propylene	C3H6(g)	42.08	20,410	62,720	266.94	48,920	45,780
Propane	C3H8(g)	44.09	-103,850	-23,490	269.91	50,350	46,360
Butane	C ₄ H ₁₀ (g)	58.12	-126,150	-15,710	310.03	49,500	45,720
Pentane	C ₅ H ₁₂ (g)	72.15	-146,440	-8,200	348.40	49,010	45,350
Octane	C ₈ H ₁₈ (g)	114.22	-208,450	17,320	463.67	48,260	44,790
Octane "	C ₈ H ₁₈ (1)	114.22	-249,910	6,610	360.79	47,900	44,430
Benzene	C ₆ H ₆ (g)	78.11	82,930	129,660	269.20	42,270	40,580
Methyl alcohol	CH ₃ OH(g)	32.04	-200,890	-162,140	239.70	23,850	21,110
Methyl alcohol	CH ₃ OH(I)	32.04	-238,810	-166,290	126.80	22,670	19,920
Ethyl alcohol	C2H3OH(g)	46.07	-235,310	-168,570	282.59	30,590	27,720
Ethyl alcohol	C2H3OH(1)	46.07	-277,690	174,890	160.70	29,670	26,800

Source: Based on JANAF Thermochemical Tables, NSRDS-NBS-37, 1971; Selected Values of Chemical Thermodynamic Properties, NBS Tech. Note 270-3, 1968; and API Research Project 44, Carnegie Press, 1953. Heating values calculated.

[Table 1]

ideal-gas spe	cific heats	of various	us common gases (C	'ancluded)				
(c) As a func	tion of tem	perature						
			<u>c</u> =	$a + bT + cT^2 + dT^3$				
				K, c _p in kJ/kmol-K)				
1						E MOTOR SERVICE	% error	
Substance	Formula		ь	c	ď	Temperature range, K	Max.	Avg
Nitrogen	N ₂	28.90	-0.1571×10^{-2}	0.8081 × 10 ⁻⁹	-2.873 × 10 ⁻⁹	273-1800	0.59	0.34
Oxygan	O ₂	25.48	1.520×10^{-2}	-0.7155×10^{-5}	1.312 × 10-9	273-1800	1.19	0.26
Air	_	28.11	0.1967 × 10 ⁻²	0.4802×10^{-5}	-1.966 × 10-9	273-1800	0.72	0.33
Hydrogen	H ₂	29.11	-0.1916 × 10-2	0.4003 × 10 ⁻⁵	-0.8704 × 10-9	273-1800	1.01	0.2
Carbon	100							0.20
monoxide Carbon	CO	28.16	0.1675×10^{-2}	0.5372 × 10 ⁻⁶	-2.222×10^{-9}	273-1800	0.89	0.3
dioxide	CO.	22.26	5.981 × 10 ⁻²	-3.501×10^{-5}	7.469 × 10-*	273-1800	0.67	0.2
Water vapor	H ₂ Ô	32.24	0.1923 × 10-2	1.055 × 10-5	-3.595 × 10-9	273-1800	0.53	0.24
Nitric oxide	NO:	29.34	-0.09395×10^{-2}	0.9747×10^{-5}	-4.187 × 10-9	273-1500	0.97	0.36
Nitrous oxide Nitrogen	N ₂ O	24.11	5.8632 × 10 ⁻²	-3.562×10^{-5}	10.58 × 10-9	273-1500	0.59	0.26
dioxide	NO.	22.9	5.715 × 10 ⁻²	-3.52×10^{-6}	7.87 × 10-9	273-1500	0.46	0.18
Ammonia	NH ₂	27.568	2.5630 x 10 ⁻²	0.99072 × 10-5	-6.6909 × 10-9	273-1500	0.91	0.36
Sulfur	Sa	27.21	2.218 × 10-2	-1.628×10^{-5}	3.986 × 10 ⁻⁹	273-1800	0.99	0.38
Sulfur							0133	0.00
diexide Sulfur	SO ₂	25.78	5.795 × 10 ⁻²	-3.812 × 10 ⁻¹	8.612 × 10 ⁻⁹	273-1800	0.45	0.24
trioxide	50,	16.40	14.58 × 10 ⁻²	-11.20 × 10-5	32.42 × 10-9	273-1300	0.29	0.13
Acetylene	C ₂ H ₂	21.8	9.2143 × 10-2	-6.527×10^{-5}	18.21 × 10-9	273-1500	1.46	0.59
Benzene	C.H.	-36.22	48.475 × 10-2	-31.57 × 10 ⁻⁵	77.62 × 10-9	273-1500	0.34	0.20
Methanol	CH_O	19.0	9.152×10^{-2}	-1.22×10^{-6}	-8.039×10^{-9}	273-1000	0.18	0.08
Ethanol	C2H60	19.9	20.96×10^{-2}	-10.38×10^{-6}	20.05 × 10 ⁻⁵	273-1500	0.40	0.22
Hydrogen					Control Control Control			
chloride	HCI	30.33	-0.7620×10^{-2}	1.327×10^{-6}	-4.338 × 10 ⁻⁹	273-1500	0.22	0.08
Methane	CH ₄	19.89	5.024×10^{-2}	1.269×10^{-6}	-11.01 × 10-4	273-1500	1.33	0.57
Ethane	C2H6	6,900	17.27×10^{-2}	-6.406 × 10 ⁻⁵	7.285 × 10 ⁻⁹	273-1500	0.83	0.28
Propane	C ₃ H ₆	-4.04	30,48 × 10 ⁻²	-15.72×10^{-5}	31.74 × 10 ⁻⁹	273-1500	0.40	0.12
n-Butane	C ₄ H ₁₀	3.96	37.15 × 10 ⁻⁸	-18.34×10^{-5}	35.00×10^{-9}	273-1500	0.54	0.24
Butane	C4H10	-7.913	41.60×10^{-2}	-23.01×10^{-6}	49.91 × 10 ⁻⁹	273-1500	0.25	0.13
n-Pentane	C ₆ H ₁₂	6,774	45.43 × 10 ⁻²	-22.46 × 10 ⁻⁵	42.29 × 10 ⁻⁹	273-1500	0.56	0.21
n-Hexane	CeH14	6.938	55.22 × 10 ⁻²	-28.65×10^{-6}	57.69 × 10 ⁻⁹	273-1500	0.72	0.20
Ethylene	C2H4	3.95	15.64 × 10-2	-8.344×10^{-5}	17.57 × 10 ⁻⁹	273-1500	0.54	0.13
Propylene	C ₃ H ₆	3.15	23.83 × 10-2	-12.18×10^{-6}	24.62 × 10-9	273-1500	0.73	0.17

Table A-2 from Thermodynmaics by Y.A. Cengel and M.A. Boles, 7^{th} edition, McGraw Hill, 2011. Here, the universal gas constant = \overline{R} = 8314 J/kmolK

[Table 2]