

Project 3.

Due date: Wednesday November 21, 2018

General Information:

This project deals with analysis of the hybrid solar fossil-fuel gas turbine system in the figures below. You may team up with a partner for this project. Do not share information or results with other groups.

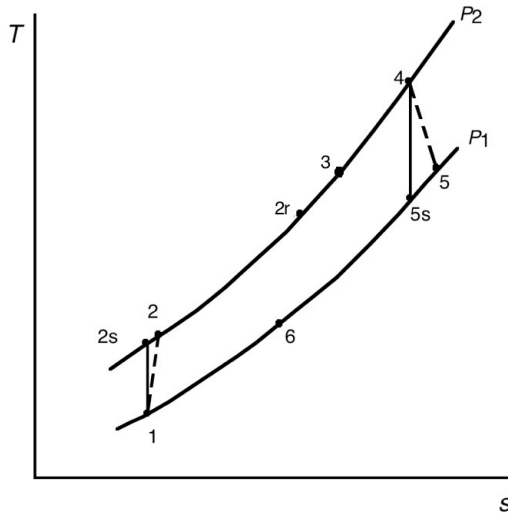


Figure 1.

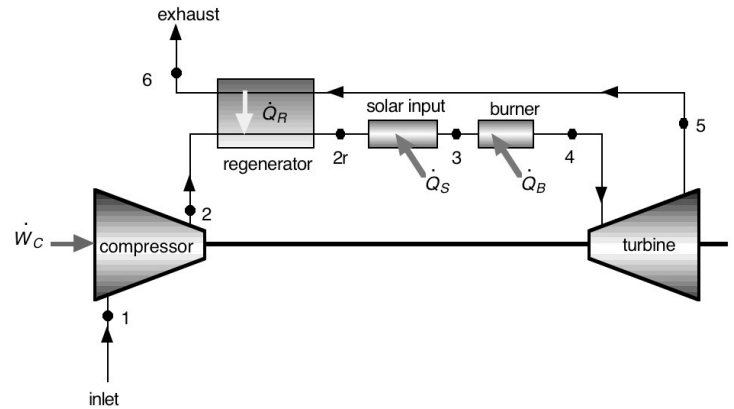


Figure 2.

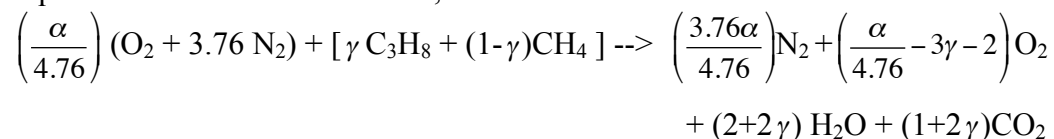
The objective of this project is to construct a computer simulation of the performance of the gas turbine system shown in Figures 1 and 2 above. Air at atmospheric pressure $P_1 = 101$ kPa and at a temperature T_1 equal to 25 °C enters the inlet at a flow rate of 6.0 kg/s. Treat air as an ideal gas with an effective molecular mass \bar{M} of 28.97 kg/kmol.

Task 1. In the burner, a mixture of propane (C_3H_8) and methane (CH_4) will be injected into the airflow and burned. Key parameters here are the molar air-to-fuel ratio α and the fuel propane mole fraction γ defined as.

$$\alpha = (\text{moles of air})/(\text{moles of propane and methane mixture}) \text{ in inlet flow to burner}$$

$$\gamma = (\text{moles of propane})/(\text{moles of propane and methane in fuel mixture})$$

A stoichiometric mixture has just enough oxygen in the air to convert all the propane and methane to H_2O and CO_2 , with no oxygen left over. For arbitrary γ and a value of α greater than or equal to the stoichiometric value, the balanced chemical reaction can be written as



Note that the above equation scales the number of moles of other species on a per mole of fuel mixture basis. For stoichiometric conditions,

$$\alpha = \alpha_{stoich} = 4.76(2 + 3\gamma)$$

The main objective of this first task is to write a computer program to determine the molar air-to-fuel ratio α that will result in a specified combustor adiabatic flame (exit) temperature T_{af} for given reactant temperature T_r . By definition, the adiabatic flame temperature T_{af} is the temperature of the products that satisfies the combustor energy balance with no heat interaction:

$$\sum_{reactants} \dot{n}_r \hat{h}_r = \sum_{products} \dot{n}_p \hat{h}_p$$

Based on this requirement, your computer program should find the value of the molar air-to-fuel ratio α that will satisfy the following equation for specified reactant temperature T_r and product temperature T_p :

$$\begin{aligned} \left(\frac{\alpha}{4.76} \right) \hat{h}_{O_2}(T_r) + \left(\frac{3.76\alpha}{4.76} \right) \hat{h}_{N_2}(T_r) + \gamma \hat{h}_{C_3H_8}(T_r) + (1-\gamma) \hat{h}_{CH_4}(T_r) &= \left(\frac{3.76\alpha}{4.76} \right) \hat{h}_{N_2}(T_p) \\ &+ \left(\frac{\alpha}{4.76} - 3\gamma - 2 \right) \hat{h}_{O_2}(T_p) + (2+2\gamma) \hat{h}_{H_2O}(T_p) + (1+2\gamma) \hat{h}_{CO_2}(T_p) \end{aligned} \quad (1)$$

In this relation, for each gas species i at temperature T , calculate the molar enthalpy from the heat of formation and the specific heat:

$$\hat{h}_i(T) = \hat{h}_i^\circ(T^\circ) + \hat{c}_{p,i}(T_{avg})(T - T^\circ) \quad \text{where } T_{avg} = 0.5(T_r + T_p) \quad (2)$$

In the exhaust gas, assume water exists as water vapor. Rearranging Eq. (1) to solve for the air-to-fuel ratio yields

$$\alpha = \frac{4.76 \left[-\gamma \hat{h}_{C_3H_8}(T_r) - (1-\gamma) \hat{h}_{CH_4}(T_r) - (3\gamma + 2) \hat{h}_{O_2}(T_p) + (2+2\gamma) \hat{h}_{H_2O}(T_p) + (1+2\gamma) \hat{h}_{CO_2}(T_p) \right]}{\left[\hat{h}_{O_2}(T_r) + 3.76 \hat{h}_{N_2}(T_r) - 3.76 \hat{h}_{N_2}(T_p) - \hat{h}_{O_2}(T_p) \right]} \quad (3)$$

Note that this relation (3) applies only for $T_{af} < T_{af,stoich}$ and $\alpha > \alpha_{stoich}$.

Write a computer program to find the value of the molar air-to-fuel ratio α that will result in a product temperature T_p for specified reactant temperature T_r . (Note that here we take the regenerator heated air and injected fuel to be at the same temperature.) To do this the program must use Eq. (3) with the specified T_r , T_p and γ . Incorporate the following features in the program:

- (a) To evaluate $\hat{c}_{p,i}$ for each species in the enthalpy computation (2), use the appropriate relation for molar specific heat from the attached table, evaluated at $T_{avg} = 0.5(T_r + T_p)$.

- (b) Use the appropriate values of the heat of formation $\hat{h}_i^\circ(T^\circ)$ at reference temperature $T^\circ = 25^\circ\text{C}$ provided in the attached table.

When it is completed, use your program to determine the molar air-to-fuel ratio α that results in a product temperature of 1900 K for (i) pure propane, (ii) pure methane, and (iii) a 50% mole fraction mixture. Take the inlet reactant temperature to be 550 K for all three cases. Summarize your results in a table.

Task 2. Write a computer program to compute the exit condition from the compressor and the work required per kilogram of air. For this computation,

- (i) Guess the exit temperature T_2 ,
- (ii) Compute \hat{c}_p at the average temperature for the process $T_{avg} = 0.5(T_1 + T_2)$ using the relation for \hat{c}_p (kJ/kmolK) as a function of T (K) for air in the table provided on page 7. (For air, take the molar enthalpy to be zero at $T_1 = 25^\circ\text{C}$.)
- (iii) Compute $\hat{c}_v = \hat{c}_p - \bar{R}$ and use a constant \hat{c}_p and \hat{c}_v analysis to compute the enthalpy \hat{h}_2 per kmol of air and the temperature at the exit from the compressor T_2 . Recompute the average temperature using the newly computed T_2 value and repeat the calculation of the outlet condition. Terminate the iterative calculation when successive T_2 values agree within 0.2°C .

Set-up the computer code for this Task (preferably as function) so that different values of P_2 and compressor efficiency η_{comp} can be specified as input to the computation.

Task 3.

In the burner, a mixture of propane (C_3H_8) and methane (CH_4) will be injected into the airflow and burned. The design value of the mole fraction of C_3H_8 in the fuel mixture, γ , is 0.25. (a) Using the chemical reaction for this propane and methane mixture with air ($\text{O}_2 + 3.76 \text{ N}_2$) with possible products being CO_2 , H_2O , O_2 and N_2 , derive relations for the mole fraction of each exhaust gas species as a function of molar air to fuel ratio α . (b) Set up a computer program (preferably as a function) to compute $\hat{c}_{p,prod}$ for the product gas mixture as the mole-fraction weighed average of the \hat{c}_p values for the individual species

$$\hat{c}_{p,prod} = y_{\text{H}_2\text{O}} \hat{c}_{p,\text{H}_2\text{O}} + y_{\text{CO}_2} \hat{c}_{p,\text{CO}_2} + y_{\text{N}_2} \hat{c}_{p,\text{N}_2} + y_{\text{O}_2} \hat{c}_{p,\text{O}_2}$$

In this relation, use the pure gas relations from the table provided on page 7. For stoichiometric combustion of the fuel mixture, evaluate $\hat{c}_{p,prod}$ for the product gases at 600 K and compare it to \hat{c}_p for pure air at the same temperature.

Task 4.

Construct a system analysis computer program to execute the following steps for specified P_1 , T_1 , P_2 , T_4 , γ , \dot{Q}_s , η_{comp} , η_{turb} , and ϵ_{regen} :

- (i) Use the iterative scheme developed in Task 2 to determine the temperature and air molar enthalpy at state 2. (Note: Set the enthalpy \hat{h}_1 at state 1 equal to 0.0 kJ/kmol and determine enthalpies at other states by determining the change in enthalpy for each process.)

(ii) In Task 3 you used the chemical reaction for propane (C_3H_8) and methane (CH_4) and air ($O_2 + 3.76 N_2$), with possible products being CO_2 , H_2O , O_2 and N_2 , to derive relations for the mole fraction of each exhaust gas species as a function of molar air to fuel ratio α . Implement these in your system analysis program. In the first iteration, take the value of α to be α_{stoich} , the molar air to fuel ratio at stoichiometric conditions in the burner.

(iii) Guess $T_5 = T_{5,guess}$

(iv) Compute $\hat{c}_{p,prod}$ at the average temperature for the turbine expansion process $T_{avg} = 0.5(T_4 + T_{5,guess})$. Take the value of α to be α_{stoich} in the first iteration, and use the value of α calculated at the end of the first iteration for the second (correction) iteration. Compute $\hat{c}_{v,prod} = \hat{c}_{p,prod} - \bar{R}$ and use a constant $\hat{c}_{p,prod}$ analysis to compute the molar enthalpy change $\hat{h}_4 - \hat{h}_5$ per kmol of gas and the temperature T_5 at the exit from the turbine. Compute the error $E = T_5 - T_{5,guess}$. If $|E|$ is less than $0.2^\circ C$, the system computation is complete. If $|E|$ is not less than $0.2^\circ C$, iterate T_5 until the condition is satisfied. Note that if you program the steps in this task into a function, in MATLAB you can use a root solver to find the value of T_5 that makes E zero.

(v) For the regenerator, evaluate the \hat{c}_p for the air and $\hat{c}_{p,prod}$ for the product gases at $T_{avg} = 0.5(T_2 + T_5)$. For the product gases, use the appropriate α value, as described in step (iv). Then compute T_{2r} for specified regenerator effectiveness ϵ_{regen} by solving:

$$\epsilon_{regen} = \frac{\dot{n}\hat{c}_{p,air}(T_{2r} - T_2)}{(\dot{n}\hat{c}_p)_{min}(T_5 - T_2)}$$

where $(\dot{n}\hat{c}_p)_{min}$ is the minimum of $\{(\dot{n}\hat{c}_p)_{air}, (\dot{n}\hat{c}_p)_{prod}\}$. Note that \dot{n}_{prod} is the kmol per second of product gases flowing as a result of burning the propane/methane fuel mixture to achieve the specified α for the air flow of 6.0 kg/s .

(vi) For solar heat input \dot{Q}_{solar} , determine the temperature at T_3 from a steady-flow energy balance (First Law).

(vii) Use the computer code developed in Task 1 to compute α (using Eq. (3)) from T_3 , and T_4 .

(viii) Repeat steps (ii)-(vii) using the α value determined in the previous step to evaluate the product gas mole fractions and specific heats in steps (ii), (v), (vi). The resulting corrected value of α determined when repeating step (vi) may be taken as the solution.

(ix) When the corrected (second iteration) version of α is determined, compute the system (cycle) net power output, the heat input in the combustor, and the efficiency of the cycle.

When the program is functional, run the computation for $\gamma = 0.25$, $\dot{Q}_s = 0$, $P_2 = 500 \text{ kPa}$, $T_4 = 1600 \text{ K}$, $\eta_{comp} = 0.85$, $\eta_{turb} = 0.85$, $\epsilon_{regen} = 0.75$ and compare the resulting efficiency to that

predicted by the constant specific heat relation derived in class. Present your comparison in a table.

Task 5. For this Task, consider a system with $\eta_{comp} = 0.85$, $\eta_{turb} = 0.85$, $\epsilon_{regen} = 0.75$, $P_2 = 500$ kPa, $\gamma = 0.25$, and $T_4 = 1600$ K. Because the incident angle of the sun's rays varies with time over the peak collection hours of the day, \dot{Q}_s varies from 2.0 to 3.0 MW over the peak collection period of the daytime (and, of course, \dot{Q}_s is zero at night).

(a) Use your program to determine the value of α required to attain $T_4 = 1600$ K, for \dot{Q}_s values of 0, 2.0 MW, 2.5 MW, and 3.0 MW. Also determine the resulting variations of the net power output, the heat input in the combustor, and the efficiency of the cycle. Summarize your results in appropriate tables, and plot the resulting variations of these parameters with \dot{Q}_s over this range.

(b) If the mole fraction of propane (γ) in the fuel increases to 0.5 or decreases to 0, how will the system performance change? Briefly discuss the reasons for your answers.

(c) (ME246 students only) Do you think that changing the system to input the combustion heat before the solar heat input would be advantageous? Discuss the reasons for your answer in a brief paragraph.

Tasks to be divided between coworkers:

- (1) Assemble the analysis and program for the compressor analysis
- (2) Assemble the analysis relations for system model program
- (3) Program development for the system analysis (flow chart and coding)
- (5) Analysis of the results
- (6) Write-up of the results and conclusions

Deliverables:

Written final report should include:

- (1) Written summary of how the work was divided between coworkers.
- (2) Documentation of relations used to analyze processes in the system and a summary of idealizations used.
- (3) A flow chart or algorithm summary for the program used must be submitted. Reasoning behind the program structure should be described.
- (4) Assess results relative to simpler constant specific heat model.
- (5) Document results in tables and plots. Describe and discuss the computed results in Task 5. Provide clear answers to parts (b) and (c) in Task 5. A copy of your program should be attached to the report as an appendix. **(Due 11/21/18)**

Grade will be based on:

- (1) thoroughness of documentation of your analysis
- (2) accuracy and clarity of interpretation
- (3) thoroughness of the design parameter investigations and the documentation of the reasons for your design recommendations, and assessments.

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

Substance	Formula	Molar Mass, M (kg/kmol)	Enthalpy of Formation, \bar{h}_f° (kJ/kmol)	Gibbs Function of Formation, \bar{g}_f° (kJ/kmol)	Absolute Entropy, \bar{s}° (kJ/kmol · K)	Heating Values	
						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	N ₂ (g)	28.01	0	0	191.50	—	—
Oxygen	O ₂ (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	C ₂ H ₂ (g)	26.04	226,730	209,170	200.85	49,910	48,220
Ethylene	C ₂ H ₄ (g)	28.05	52,280	68,120	219.83	50,300	47,160
Ethane	C ₂ H ₆ (g)	30.07	−84,680	−32,890	229.49	51,870	47,480
Propylene	C ₃ H ₆ (g)	42.08	20,410	62,720	266.94	48,920	45,780
Propane	C ₃ H ₈ (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 (l)	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(l)	32.04	−238,810	−166,290	126.80	22,670	19,920
Ethyl alcohol	C ₂ H ₅ OH(g)	46.07	−235,310	−168,570	282.59	30,590	27,720
Ethyl alcohol	C ₂ H ₅ OH(l)	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 A-2

Ideal-gas specific heats of various common gases (Concluded)

(c) As a function of temperature

$$\bar{c}_p = a + bT + cT^2 + dT^3$$

(T in K, c_p in kJ/kmol·K)

Substance	Formula	a	b	c	d	Temperature range, K	% error	
							Max.	Avg.
Nitrogen	N ₂	28.90	-0.1571×10^{-2}	0.8081×10^{-5}	-2.873×10^{-9}	273–1800	0.59	0.34
Oxygen	O ₂	25.48	1.520×10^{-2}	-0.7155×10^{-5}	1.312×10^{-9}	273–1800	1.19	0.28
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	0.26
Carbon monoxide	CO	28.16	0.1675×10^{-2}	0.5372×10^{-5}	-2.222×10^{-9}	273–1800	0.89	0.37
Carbon dioxide	CO ₂	22.26	5.981×10^{-2}	-3.501×10^{-5}	7.469×10^{-9}	273–1800	0.67	0.22
Water vapor	H ₂ O	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	N ₂ O	24.11	5.8632×10^{-2}	-3.562×10^{-5}	10.58×10^{-9}	273–1500	0.59	0.26
Nitrogen dioxide	NO ₂	22.9	5.715×10^{-2}	-3.52×10^{-5}	7.87×10^{-9}	273–1500	0.46	0.18
Ammonia	NH ₃	27.568	2.5630×10^{-2}	0.99072×10^{-5}	-6.6909×10^{-9}	273–1500	0.91	0.36
Sulfur	S ₂	27.21	2.218×10^{-2}	-1.628×10^{-5}	3.986×10^{-9}	273–1800	0.99	0.38
Sulfur dioxide	SO ₂	25.78	5.795×10^{-2}	-3.812×10^{-5}	8.612×10^{-9}	273–1800	0.45	0.24
Sulfur trioxide	SO ₃	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 ₆ H ₆	-36.22	48.475×10^{-2}	-31.57×10^{-5}	77.62×10^{-9}	273–1500	0.34	0.20
Methanol	CH ₄ O	19.0	9.152×10^{-2}	-1.22×10^{-5}	-8.039×10^{-9}	273–1000	0.18	0.08
Ethanol	C ₂ H ₆ O	19.9	20.96×10^{-2}	-10.38×10^{-5}	20.05×10^{-9}	273–1500	0.40	0.22
Hydrogen chloride	HCl	30.33	-0.7620×10^{-2}	1.327×10^{-5}	-4.338×10^{-9}	273–1500	0.22	0.08
Methane	CH ₄	19.89	5.024×10^{-2}	1.269×10^{-5}	-11.01×10^{-9}	273–1500	1.33	0.57
Ethane	C ₂ H ₆	6.900	17.27×10^{-2}	-6.406×10^{-5}	7.285×10^{-9}	273–1500	0.83	0.28
Propane	C ₃ H ₈	-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^{-2}	-18.34×10^{-5}	35.00×10^{-9}	273–1500	0.54	0.24
i-Butane	C ₄ H ₁₀	-7.913	41.60×10^{-2}	-23.01×10^{-5}	49.91×10^{-9}	273–1500	0.25	0.13
n-Pentane	C ₅ H ₁₂	6.774	45.43×10^{-2}	-22.46×10^{-5}	42.29×10^{-9}	273–1500	0.56	0.21
n-Hexane	C ₆ H ₁₄	6.938	55.22×10^{-2}	-28.65×10^{-5}	57.69×10^{-9}	273–1500	0.72	0.20
Ethylene	C ₂ H ₄	3.95	15.64×10^{-2}	-8.344×10^{-5}	17.67×10^{-9}	273–1500	0.54	0.13
Propylene	C ₃ H ₆	3.15	23.83×10^{-2}	-12.18×10^{-5}	24.62×10^{-9}	273–1500	0.73	0.17

Source: B. G. Kyle, *Chemical and Process Thermodynamics* (Englewood Cliffs, NJ: Prentice-Hall, 1984). Used with permission.

Table A-2 from Thermodynamics by Y.A. Cengel and M.A. Boles, 7th edition, McGraw Hill, 2011.
Here, the universal gas constant = $\bar{R} = 8314 \text{ J/kmol·K}$