

Example Problem- Adiabatic Flame Temperature for Methane-Air								
(a)	Heat of Reaction Method			CH4 + 2O2 = CO2 + 2H2O(g)				
	Cp coefficients (kJ/gmol-K)			Basis: 1 mol CH4				
		a	b	c	d	T	Form	DelH_f
	CH4	3.43E-02	5.47E-05	3.66E-09	-1.10E-11	C	1	-74.85
	O2	2.91E-02	1.16E-05	-6.08E-09	1.31E-12	C	1	0
	N2	2.90E-02	2.20E-06	5.72E-09	-2.87E-12	C	1	0
	CO2	3.61E-02	4.23E-05	-2.89E-08	7.46E-12	C	1	-393.5
	H2O(g)	3.35E-02	6.88E-06	7.60E-09	-3.59E-12	C	1	-241.83
	Heat of reaction =		-8.02E+02 kJ/mol CH4					
	Guess: T_ad=		2000 C		2273.0	K		
		Out						
		T(C)	n	Int Cp dT	H			
	CH4	2.00E+03	0		0.00E+00			
	O2	2.00E+03	0		0.00E+00			
	N2	2.00E+03	7.524	6.54E+01	4.92E+02			
	CO2	2.00E+03	1.0	1.09E+02	1.09E+02			
	H2O	2.00E+03	2.0	8.57E+01	1.71E+02			
				Sum=	7.73E+02	kJ		
	$Q = 0 = \Delta H_{rxn} + \left(\sum n_i \int_{25}^T C_{p,i} dT \right)_{products}$							
	Q=		-2.96E+01 kJ		Use solver to change T to set this Q to 0			

Example Problem- Adiabatic Flame Temperature for Methane-Air									
(b)	Hout - Hin Method				CH4 + 2O2 = CO2 + 2H2O(g)				
	Cp coefficients (kJ/gmol-K)				Basis: 1 mol CH4				
		a	b	c	d	T	Form	DelH_f	
	CH4	3.43E-02	5.47E-05	3.66E-09	-1.10E-11	C	1	-74.85	
	O2	2.91E-02	1.16E-05	-6.08E-09	1.31E-12	C	1	0	
	N2	2.90E-02	2.20E-06	5.72E-09	-2.87E-12	C	1	0	
	CO2	3.61E-02	4.23E-05	-2.89E-08	7.46E-12	C	1	-393.5	
	H2O(g)	3.35E-02	6.88E-06	7.60E-09	-3.59E-12	C	1	-241.83	
	Guess: T_ad=		2000 C		2273.0	K			
		In				Out			
		T(C)	n	Hhat	H	T(C)	n	Hhat	H
	CH4	25	1	-7.49E+01	-7.49E+01	2000.0	0		0.00E+00
	O2	25	2	0.00E+00	0.00E+00	2000.0	0		0.00E+00
	N2	25	7.524	0.00E+00	0.00E+00	2000.0	7.524	6.54E+01	4.92E+02
	CO2	25	0			2000.0	1	-2.85E+02	-2.85E+02
	H2O	25	0			2000.0	2	-1.56E+02	-3.12E+02
				Sum=	-7.49E+01			Sum=	-1.04E+02 kJ
	$Q = 0 = \left(\sum n_i \hat{H}_i \right)_{out} - \left(\sum n_i \hat{H}_i \right)_{in}$								
	Q= -2.96E+01 kJ				Use solver to change T to set this Q to 0				

Example Problem- Adiabatic Flame Temperature for Methane-Air

(a) **Heat of Reaction Method (Path Method)** $\text{CH}_4 + 2\text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O(g)}$

Cp coefficients (kJ/gmol-K)				Basis: 1 mol CH ₄			
	a	b	c	d	T	Form	DelH _f
CH ₄	3.43E-02	5.47E-05	3.66E-09	-1.10E-11	C	1	-74.85
O ₂	2.91E-02	1.16E-05	-6.08E-09	1.31E-12	C	1	0
N ₂	2.90E-02	2.20E-06	5.72E-09	-2.87E-12	C	1	0
CO ₂	3.61E-02	4.23E-05	-2.89E-08	7.46E-12	C	1	-393.5
H ₂ O(g)	3.35E-02	6.88E-06	7.60E-09	-3.59E-12	C	1	-241.83

Heat of reaction = -8.02E+02 kJ/mol CH₄

Guess: T_{ad} = 2000 C

2273.0 K

Out

T(C) n Int Cp dT H

CH₄ 2.00E+03 0 0.00E+00

O₂ 2.00E+03 0 0.00E+00

N₂ 2.00E+03 7.524 6.54E+01 4.92E+02

CO₂ 2.00E+03 1.0 1.09E+02 1.09E+02

H₂O 2.00E+03 2.0 8.57E+01 1.71E+02

Sum= 7.73E+02 kJ

$$Q = 0 = \Delta H_{rxn} + \left(\sum n_i \int_{25}^T C_{p,i} dT \right)_{\text{products}}$$

Q= -2.96E+01 kJ Use solver to change T to set this Q to 0

with no N₂

T

Q

3000 -361

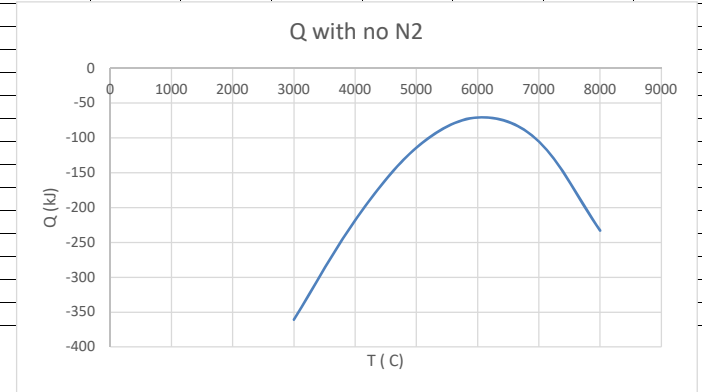
4000 -218

5000 -114

6000 -70.7

7000 -105

8000 -233



Example Problem- Adiabatic Flame Temperature for Methane-Air										
(b) Hout - Hin Method										
	Cp coefficients (kJ/gmol-K)									
		a	b	c	d			T	Form	DelH_f
	CH4	0.0120541	8.573E-05	-3.199E-08	5.745E-12	-4.678E-16	1.243E-20	K	J	-74.85
	O2	0.0252337	1.587E-05	-8.678E-09	2.646E-12	-3.902E-16	2.175E-20	K	J	0
	N2	0.02732989	5.033E-06	1.001E-09	-1.074E-12	2.276E-16	-1.521E-20	K	J	0
	CO2	0.02342203	5.607E-05	-3.370E-08	1.001E-11	-1.428E-15	7.807E-20	K	J	-393.5
	H2O(g)	0.03146368	3.956E-06	9.979E-09	-5.213E-12	9.602E-16	-6.079E-20	K	J	-241.83
	Guess: T_ad=		2000 C		2273.0	K				
		In				Out				
		T(K)	n	Hhat	H	T(K)	n	Hhat	H	
	CH4	298	1	-7.49E+01	-7.49E+01	2273.0	0		0.00E+00	
	O2	298	2	0.00E+00	0.00E+00	2273.0	0		0.00E+00	
	N2	298	7.524	0.00E+00	0.00E+00	2273.0	7.524	6.59E+01	4.96E+02	
	CO2	298	0			2273.0	1	-2.85E+02	-2.85E+02	
	H2O	298	0			2273.0	2	-1.55E+02	-3.10E+02	
				Sum=	-7.49E+01			Sum=	-9.97E+01	kJ
	$Q = 0 = \left(\sum n_i \hat{H}_i \right)_{out} - \left(\sum n_i \hat{H}_i \right)_{in}$									
	Q= -2.49E+01 kJ		Use solver to change T to set this Q to 0							

Example Problem- Adiabatic Flame Temperature								40 mol% CO, 60 mol% H ₂		
Basis: 100 moles of fuel, using JANAF Cp's										
(a)	Cp coefficients (cal/gmol-K)									
		a	b	c	d			T	Form	DelH_f
	CO	6.401	1.77E-03	-2.24E-07	-1.01E-10	3.09E-14	-2.32E-18	K	Janaf	-110.52
	H2	7.011	-6.83E-04	1.35E-06	-4.96E-10	7.69E-14	-4.36E-18	K	Janaf	0
	O2	6.031	3.79E-03	-2.07E-06	6.32E-10	-9.33E-14	5.20E-18	K	Janaf	0
	N2	6.532	1.20E-03	2.39E-07	-2.57E-10	5.44E-14	-3.64E-18	K	Janaf	0
	CO2	5.598	1.34E-02	-8.05E-06	2.39E-09	-3.41E-13	1.87E-17	K	Janaf	-393.5
	H2O(g)	7.52	9.45E-04	2.39E-06	-1.25E-09	2.30E-13	-1.45E-17	K	Janaf	-241.83
		T_init=	2.98E+02 K							
	Guess: T_ad=		1500 K	1227.0	C			$Q = 0 = \left(\sum n_i \hat{H}_i \right)_{out} - \left(\sum n_i \hat{H}_i \right)_{in}$		
	In									
	T(C)	n		H_hat	H					
	CO	25	40	-110.52	-4.42E+03					
	H2	25	60	0	0.00E+00					
	O2	25	50	0	0.00E+00					
	N2	25	188	0	0.00E+00					
	CO2		0	-393.5	0.00E+00					
	H2O		0							
			Sum=		-4.42E+03 kJ					
	Out									
	T(C)	n		H_hat	H					
	CO	1.50E+03	0		0.00E+00					
	H2	1.50E+03	0		0.00E+00					
	O2	1.50E+03	0	4.06E+01	0.00E+00					
	N2	1.50E+03	188	3.84E+01	7.22E+03					
	CO2	1.50E+03	40	-3.32E+02	-1.33E+04					
	H2O	1.50E+03	60	-1.94E+02	-1.16E+04					
			Sum=		-1.77E+04 kJ					
	Q=					-1.33E+04 kJ	Use solver to set this to 0 by changing the temperature			