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) — 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**

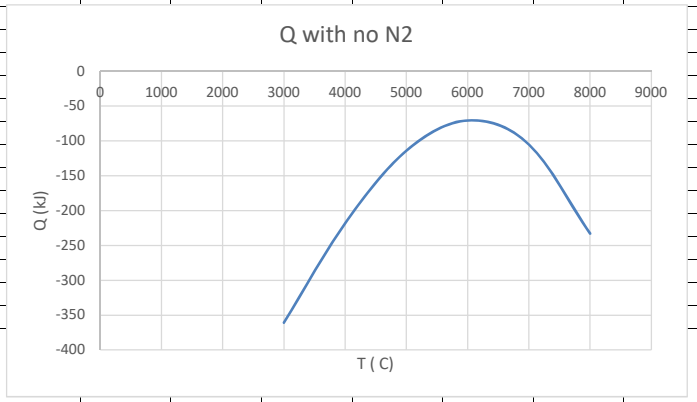
Guess: T_ad= 2000 C 2273.0 K

	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

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