Heat of combustion, Δh_c

is numerically same as enthalpy of reaction (Δh_R) with the opposite sign $\boxed{\Delta h_c = -\Delta h_R}$

Upper/higher heating value (HHV) is the Δh_c, assuming all the water in the product is condensed to liquid phase.

Lower heating value (LHV) is Δh_c when none of the water is assumed to be condensed.

$$HHV > LHV$$

(5–12% depends fuel)

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Example problem: heating values

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

Determine the upper and lower heating values at 298 K of gaseous n-decane, $C_{10}H_{22}$, per Kmol and Kg of fuel. The molecular weight of n-decane is 142 g/mol.

Ex. prob. 2.4 from Turns. (1)

For complete combustion of n-decane, $C_{10}H_{22}$

$x = 10,\ y = 22,\ \Rightarrow a = x + y/4 = 10 + \frac{22}{4} = 15.5$

Chemical equation is.

$$C_{10}H_{22}(g) + 15.5(O_2 + 3.76 N_2) \longrightarrow 10\, CO_2(g) + 11\, H_2O + 58.28\, N_2(g)$$

Heat of Combustion, $\Delta H_c = -\Delta H_R = -(H_{prod} - H_{reac})$

$$\Delta H_c = H_{reac} - H_{prod}$$

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Example problem

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

The following are obtained from the tables,

$$h^{\circ}_{f\,C_{10}H_{22}(g)} = -249659 \text{ kJ/kmol}$$

$$h^{\circ}_{f\,O_2(g)} = h^{\circ}_{f\,N_2(g)} = 0$$

$$h^{\circ}_{f\,CO_2(g)} = -393546 \text{ kJ/kmol}$$

$$h^{\circ}_{f\,H_2O(g)} = -241845 \text{ kJ/kmol}$$

Lower Heating Value (LHV).

$$H_{reac} = 1 \times h^{\circ}_{f\,C_{10}H_{22}(g)} + 15.5 \times \left(h^{\circ}_{f\,O_2(g)} + 3.76\, h^{\circ}_{f\,N_2(g)}\right)$$

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Example problem

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

Lower Heating Value (LHV).

$$H_{reac} = 1 \times h^{\circ}_{f\,C_{10}H_{22}(g)} + 15.5 \times \left(h^{\circ}_{f\,O_2(g)} + 3.76\, h^{\circ}_{f\,N_2(g)} \right)$$

$$H_{reac} = -249659 \text{ kJ}/\cancel{\text{kmol}}$$

$$H_{prod} = 10 \times h^{\circ}_{f\,CO_2(g)} + 11 \times h^{\circ}_{f\,H_2O(g)} + 58.28 \times h^{\circ}_{f\,N_2(g)}$$

$$= 10 \times (-393546) + 11 \times (-241845) + 0$$

$$H_{prod} = -6595755 \text{ kJ}.$$

$$\Delta H_c = -249659 + 6595755 = +6346096 \text{ kJ}.$$

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Example problem

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

(2)

Since unit mole of $C_{10}H_{22}(g)$ is used,

$$\Delta h_c = 6346096 \text{ kJ/kmol}_{C_{10}H_{22}(g)}$$

$$M_{W_{C_{10}H_{22}(g)}} = 10 \times 12 + 22 \times 1 = 142 \text{ kg/kmol.}$$

$$\Rightarrow \Delta h_c = 6346096/142 = \boxed{44690.82 \text{ kJ/kg}_{C_{10}H_{22}(g)} = LHV.}$$

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Example problem

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

Higher heating value (HHV)

Here all the water have to be condensed.

$$h^\circ_{f\,H_2O(g)} = h^\circ_{f\,H_2O(l)} + h^\circ_{vap\,H_2O}$$

[h°_{vap} is the heat of vaporisation = 44010 kJ/kmol

$$h^\circ_{f\,H_2O(l)} = h^\circ_{f\,H_2O(g)} - h^\circ_{vap\,H_2O}$$

$$= -241845 - 44010 = -285855 \text{ kJ/kmol}$$

$$\therefore H_{prod} = 10 \times h^\circ_{f\,CO_2(g)} + 11 \times h^\circ_{f\,H_2O(l)} + 58.28 \times h^\circ_{f\,N_2(g)}$$

$$= 10 \times (-393546) + 11(-285855) + 0$$

$$= -7079865 \text{ kJ}.$$

Example problem

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

$$\Delta H_c = -249659 + 7079865 = 6830206 \text{ kJ}$$

$$\Delta h_c = 6830206 \text{ kJ}/\text{kmol}_{C_{10}H_{22}(g)}$$

$$\Delta h_c = \frac{6830206}{142} = \boxed{48100.04 \text{ kJ}/\text{kg}_{C_{10}H_{22}(g)} = HHV}$$

As from the lectures, $HHV_{C_{10}H_{22}(g)} > LHV_{C_{10}H_{22}(g)}$

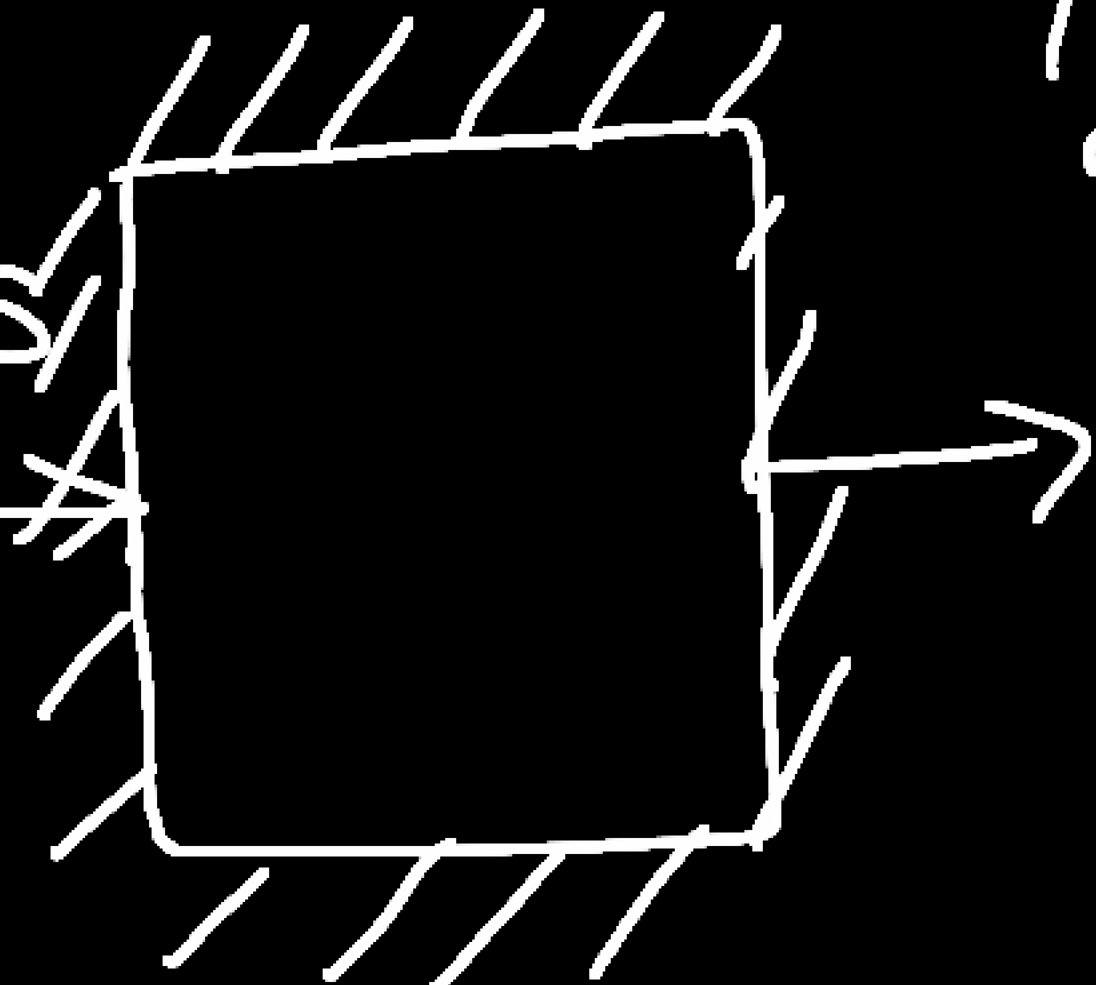
In this case, $HHV = 1.076\ LHV$.

or HHV is 7.6% higher than LHV.

Adiabatic flame temperature (T_{ad})

adiabatic / no heat transfer

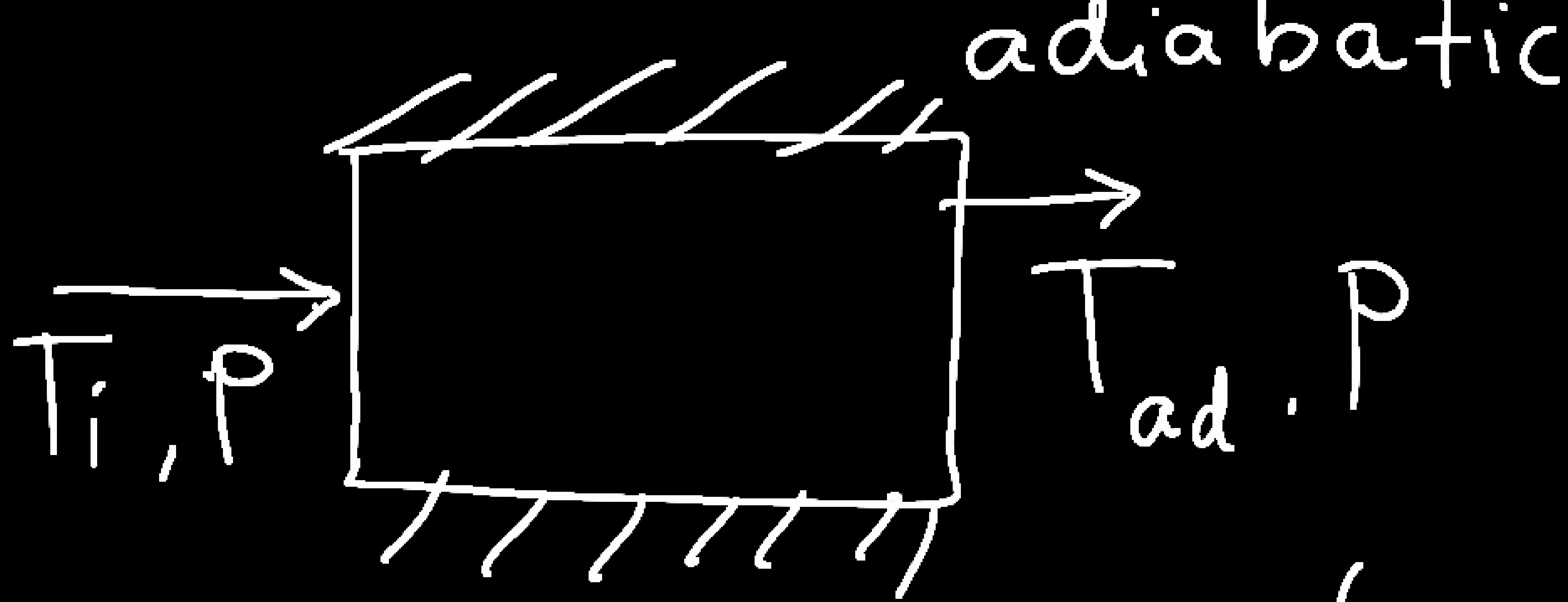
Reactants (T_i)



Product ($T_{ad} > T_i$)

Constant volume or pressure process.

Rockets / gas turbine engines.



$$H_{reac}(T_i) = H_{prod}(T_{ad})$$

"Chemical equilibrium"

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Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

Estimate the constant pressure adiabatic flame temperature for the combustion of Methane-air mixture for equivalence ratios, $\Phi = 1,\ 0.8$. The pressure is 1 atm and the initial reactant temperature is 298 K. c_p of the product mixture is evaluated at 1200 K.

Prob 2.5 (Example) from Turns. Combustion book. (1)

Combustion of Methane

$$CH_4 + 2(O_2 + 3.76\,N_2) \longrightarrow CO_2 + 2\,H_2O + 7.52\,N_2$$

From the tables, the following data are obtained.

Species	$h^\circ_{f,i}$ (kJ/kmol)	$\bar{c}_{p,i}$ (kJ/kmol-k) (@ 1200 k)
CH_4	$-74,831$	78.84
CO_2	-393546	56.21
H_2O	-241845	43.87
N_2	0	33.71
O_2	0	35.59

Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

O_2

Standardized enthalpy of reactant.

$$H_{reac}(T_{ref}) = h^\circ_{f\,CH_4} + 2h^\circ_{f\,O_2} + h^\circ_{f\,N_2} \times 7.52$$

$$= -74831 + 0 + 0.$$

$$\Rightarrow H_{reac}(T_{ref}) = -74831 \text{ kJ}.$$

For products.

$$H_{prod}(T = \cancel{298}\, T_{ad}) = h^\circ_{f\,CO_2} + \Delta h_{s\,CO_2}(T_{ad}) +$$

$$2.(h^\circ_{f\,H_2O} + \Delta h_{s\,H_2O}(T_{ad})) +$$

$$7.52(h^\circ_{f\,N_2} + \Delta h_{s\,N_2}(T_{ad}))$$

&

$$\Delta h_{s_i} = \bar{c}_{p_i}(T_{ad} - T_{ref})$$

$$= -393546 + 56.21 \times (T_{ad} - 298) +$$

$$2[-241845 + 43.87 \times (T_{ad} - 298)]$$

$$+ 7.52[0 + 33.71 \times (T_{ad} - 298)]$$

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Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

(2)

$$\Rightarrow H_{prod}(T_{ad}) = -995675.8616 + 397.4492\,T_{ad}.$$

For Adiabatic flame temperature,

$$H_{reac} = H_{prod}.$$

$$\therefore\ -74831 = -995675.8616 + 397.4492\,T_{ad}$$

$$\Rightarrow \boxed{T_{ad} = 2316.89\ K.}$$ Adiabatic flame temperature.

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Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

For fuel lean case, say $\Phi = 0.8$

$$\frac{(A/F)_s}{(A/F)} = 0.8 \Rightarrow A/F = \frac{(A/F)_s}{0.8} = \frac{17.16}{0.8} = 21.45$$

$$(A/F) = \frac{m_{air}}{m_{fuel}} = \frac{n_{air} M_{w_{air}}}{n_{fuel} M_{w_{fuel}}} = \frac{n_{air}}{n_{fuel}} \frac{28.84}{16} = 21.45$$

$$\frac{n_{air}}{n_{fuel}} = 11.9$$

For 1 mole of fuel (CH_4) $n_{fuel} = 1$

$$n_{air} = 11.9.$$

$1 (O_2 + 3.76 N_2)$ contains 4.76 moles of air.

$b (O_2 + 3.76 N_2)$ contains 11.9 moles of air

$$\Rightarrow b = \frac{11.9}{4.76} \times 1 = 2.5.$$

$\Rightarrow$

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Example: adiabatic flame temperature

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$\Rightarrow$ 4.76

So the chemical equation becomes

$$CH_4 + 2.5(O_2 + 3.76 N_2) \longrightarrow CO_2 + 2H_2O + \tfrac{1}{2}O_2 + 9.4 N_2.$$

$$H_{reac}(T_{ref}) = h^\circ_{f_{CH_4}} + 2.5\left(h^\circ_{f_{O_2}} + 3.76 \cdot h^\circ_{f_{N_2}}\right) \quad (3)$$

$$= -74831 + 2.5(0+0) = -74831 \text{ kJ}.$$

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Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

$$
\begin{aligned}
H_{prod}(T_{ad}) = {} & \bar{h}^{\circ}_{f\,CO_2} + \bar{c}_{p\,CO_2}(T_{ad} - 298) + \\
& + 2\left[\bar{h}^{\circ}_{f\,H_2O} + \bar{c}_{p\,H_2O}(T_{ad} - 298)\right] + \\
& \tfrac{1}{2}\left[\bar{h}^{\circ}_{f\,O_2} + \bar{c}_{p\,O_2}(T_{ad} - 298)\right] + \\
& 9.4\left[\bar{h}^{\circ}_{f\,N_2} + \bar{c}_{p\,N_2}(T_{ad} - 298)\right] \\
= {} & -393546 + 56.21(T_{ad} - 298) + \\
& 2\left[-241845 + 43.87(T_{ad} - 298)\right] \\
& + \tfrac{1}{2}\left[0 + 35.59(T_{ad} - 298)\right] \\
& + 9.4\left[0 + 33.71(T_{ad} - 298)\right]
\end{aligned}
$$

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Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

Equating, $H_{reac}(T_{ref}) = H_{prod}(T_{ad})$,

$$T_{ad} - 298 = 1676.5$$

$$\text{(or)}\quad T_{ad} = 1974 \text{ K.}$$

Adiabatic flame temperature decreases for $\Phi = 0.8$.

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Example: adiabatic flame temperature

An Introduction to Combustion: Concepts and Applications by Stephen R. Turns, Third Edition, Tata McGraw-Hill, New Delhi, 2012

Equating, $H_{reac}(T_{ref}) = H_{prod}(T_{ad})$,

$$T_{ad} - 298 = 1676.5$$

$$(\text{or})\quad T_{ad} = 1974\ K.$$

Adiabatic flame temperature decreases for $\Phi = 0.8$.

T_{ad} Vs ϕ

FL - flammability limits

Methane

$0.46 - 1.64$
ϕ