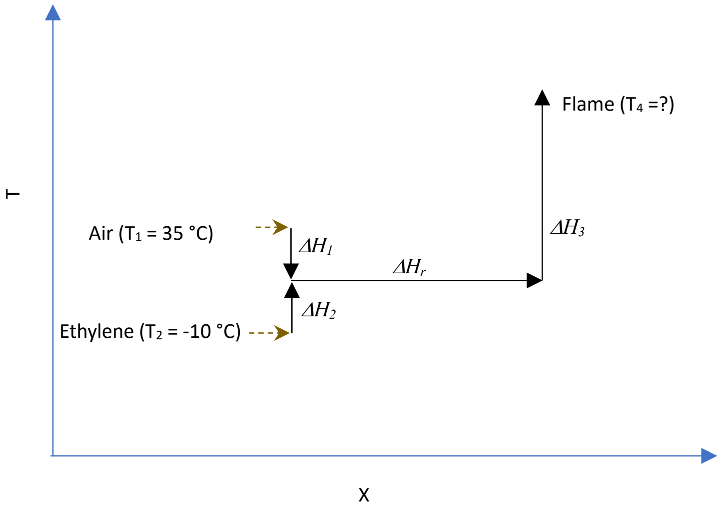
Quiz 3

Calculate the theoretical flame temperature when ethylene at -10°C is burned with 40% excess air at 35°C.

Answer:

The T-x diagram to calculate the final temperature of the reaction products is as follows:



Reaction:

$C_2H_4(g) + 3O_2(g) \rightarrow 2CO_2(g) + 2H_2O(g)$

Theoretical flame temperature means the combustion reaction goes to completion adiabatically (Q = 0) and the first law of thermodynamics is simplified into $\Delta H = 0$ (see page 153 of the textbook)

The initial temperature of air and ethylene are 35°C and -10°C. Therefore, to follow the diagram, the air must be cooled down to 25°C. ΔH for this change is negative. Ethylene must be also heated up to the same temperature (positive ΔH). Then the reaction occurs (ΔH is negative) and finally the heat released by the reaction and air increases the temperature of the products (ΔH is positive). The sum of all the enthalpy changes is zero. Because the final temperature is unknown and average C_ps of the reaction products are dependent on the final temperature, the enthalpy balance of the process is written based on an unknown final temperature. Then, the final temperature is adjusted so that $\Delta H = 0$. This can be done by trial and error, but the best method is to use the excel solver.

Basis: 1 mole of ethylene

Based on the stoichiometric coefficients of the reaction and the amount of excess air in the feed:

$n_{O_2} = 3\times1\times1.4 = 4.2$

$n_{N_2} = 3.75\times79/21 = 15.8$

For the product:

$n_{O_2} = 4.2 - (3 \times 1) = 1.2$

$n_{N_2} = 15.8$

$n_{CO_2} = 2$

$n_{H_2O} = 2$

$T_1 = 35 + 273.15 = 308.15$ K

$T_2 = -10 + 298.15$ K $= 263.15$

$T_3 = 298.15$ K

T_4 = unknown

The summary of the calculations is in the table below.

Comp.	Stoic. Coef.	Moles (ν_i)		ΔH^o_{298} (J/mol) (Page 658)	$\nu_i\ \Delta H^o_{298,\,i}$	C_p Coefficients (Page 656)				C_p of Feed (J/mol K)	ΔH of Feed (J/mol)	C_p of Product (J/mol K) (298 to T_4)	ΔH of Product (J/mol)
		Feed	Product			A	B	C	D				
Ethylene	1	1	0	52,510	-52510	1.424	1.4394E-02	-4.392E-06	0	42.55	1489.08	92.65	0.00
O_2	3	4.2	1.2	0	0	3.639	5.06E-04	0	-22700	29.48	-1237.98	34.88	73186.64
N_2	0	15.8	15.8	0	0	3.28	5.93E-04	0	4000	29.13	-4601.98	33.10	914641.44
CO_2	2	0	2	-393509	-787018	5.457	1.045E-03	0	-115700	37.53	0.00	53.98	188782.73
H_2O	2	0	2	-241818	-483636	3.47	1.45E-03	0	12100	33.60	0.00	43.15	150904.08
				$\Delta H_r = \Sigma\ \nu_i\ \Delta H^o_{298,\,i} =$	**-1323164**					$\Delta H_1 + \Delta H_2 =$	**-4350.89**	$\Delta H_3 =$	**1327514.89**

Notes:

$\Delta H_1 = \Sigma\ \nu_i\ C_{p,i}\ (298.15 - 308.15)$ (All ν_i except for ethylene)

$\Delta H_2 = \nu_{Et}\ C_{p,Et}\ (298.15 - 263.15)$

$\Delta H_3 = \Sigma\ \nu_i\ C_{p,i}\ (T_4 - 298.15)$

C_ps using Eq. 4.9 and R = 8.314 J/mol K

To determine the final temperature using excel, the C_ps of the product components are written using an initial value of T_4 which has a specific cell. Then the value of ΔH is calculated ($\Delta H = \Delta H_1 + \Delta H_2 + \Delta H_3 + \Delta H_r$). You can change the value of T_4 until ΔH = 0. To use the excel solver, choose the cell of ΔH as the objective and its value must be set to zero. Then choose the cell of T_4 as the variable cell and then click solve and then OK. (**T_4 = 2046.79 K**). After calculation make sure the value of ΔH is zero or negligible.