Clase 41 13 Oct. 2015

Título de la nota 13/10/2015

Continuando con la clase anterior se presentan los resultados del proceso irreversible de comp. Isotérmica

	Van der Waals	Berthelot	Ideal
ΔU (J/mol)	-68,2696717	-57,4147939	0
ΔH (J/mol)	-85,5186345	-35,101482	0
ΔS (J/molK)	-8,41465814	-8,64222371	-8,30865
q (J/mol)	-2524,39744	-2592,66711	-2492,595
w (J/mol)	-2456,12777	-2535,25232	-2492,595
ΔG (J/mol)	2438,87881	2557,56563	2492,595

Conclusiones

Es evidente que es necesario aplicar más trabajo para que el gas se comprima de forma irreversible; siendo mayor para el caso tipo Berthelot

El sistema se ordena más en el tipo Berthelot lo que conlleva a que $\overline{\Delta G}$ sea el menos favorable porque requiere mayor energía

El sistema tipo Berthelot resulta ser el más exotérmico; pierde más calor porque su $\overline{\Delta H} < \Delta H_{ideal} < \Delta H_{van\ der\ Waals}$

Ecuación de Avance

Redlinch - Kwong.

$$p = \frac{RT}{\bar{v}-b} - \frac{a}{\bar{v}(\bar{v}+b)T^{1/2}}$$

obtener T

$$p + \frac{a}{(\bar{v}^2+\bar{v}b)T^{1/2}} = \frac{RT}{\bar{v}-b} \qquad \frac{p(\bar{v}^2+\bar{v}b)T^{1/2}+a}{(\bar{v}^2+\bar{v}b)T^{1/2}} = \frac{RT}{\bar{v}-b}$$

reacomodando

$$\left(p\,(\bar{v}^2+\bar{v}b)\,T^{1/2}+a\right)(\bar{v}-b)=RT\left(\bar{v}^2+\bar{v}b\right)T^{1/2}$$

$$\left\{\left[p(\bar{v}^2+\bar{v}b)(\bar{v}-b)\right]T^{1/2}+a(\bar{v}-b)=RT^{3/2}(\bar{v}^2+\bar{v}b)\right\}^2$$

$$\left[p^2(\bar{v}^2+\bar{v}b)^2(\bar{v}-b)^2\right]T+\left[a(\bar{v}-b)\right]^2=R^2T^3(\bar{v}^2+\bar{v}b)^2$$

Despejando

$$T^3-T\frac{\left[p^2(\bar{v}^2+\bar{v}b)^2(\bar{v}-b)^2\right]}{R^2(\bar{v}^2+\bar{v}b)^2}-\frac{\left[a(\bar{v}-b)\right]^2}{R^2(\bar{v}^2+\bar{v}b)^2}=0$$

sustituyendo valores y checando unidades

$$T^3 - T\left[\frac{P^2(\bar{v}^2+\bar{v}b)^2(\bar{v}-b)^2}{R^2(\bar{v}^2+\bar{v}b)^2}\right] - \frac{\left[a(\bar{v}-b)\right]^2}{R^2(\bar{v}^2+\bar{v}b)^2} = 0$$

$$T^3 - T\left[\frac{P^2(\bar{v}-b)^2}{R^2}\right] - \frac{\left[a(\bar{v}-b)\right]^2}{R^2(\bar{v}^2+\bar{v}b)} = 0$$

$$K^3 - K\left[\frac{\cancel{atm^2}\,(\cancel{L/mol})^2}{\left(\frac{\cancel{atm\,L}}{\cancel{mol}\,K}\right)^2}\right] - \frac{\left(\frac{\cancel{atm}\,L^2}{mol^2}K^{1/2}\right)^2\left(\cancel{L/mol}\right)^2}{\left(\frac{\cancel{atm\,L}}{\cancel{mol}\,K}\right)^2\left[\left(\cancel{L/mol}\right)^2\right]^2} = K^3 - K^3 - K^3 = 0$$

OK correcto

Sustituyendo se obtiene

$$T^3 - 926503.29\,T - 8289.5362 = 0$$

Resolviendo se obtienen 3 raíces

$T_1 = 962.55K$ ✓ este es el resultado correcto

$T_2 = -962.55K$

$T_3 = -0.01$

Despeje de $\bar{v}$ en la ecuación de Redlinch-Kwong.

$$p = \frac{RT}{\bar{v}-b} - \frac{a}{(\bar{v}^2+\bar{v}b)T^{1/2}}$$

$$p + \frac{a}{(\bar{v}^2+\bar{v}b)T^{1/2}} = \frac{RT}{\bar{v}-b}$$

$$p(\bar{v}^2+\bar{v}b)T^{1/2} + a = \frac{RT(\bar{v}^2+\bar{v}b)T^{1/2}}{(\bar{v}-b)}$$

$$p(\bar{v}^2+\bar{v}b)T^{1/2}(\bar{v}-b) + a(\bar{v}-b) = RT^{3/2}(\bar{v}^2+\bar{v}b)$$

$$p(\bar{v}^2+\bar{v}b)T^{1/2}(\bar{v}-b)+a(\bar{v}-b)=RT^{3/2}(\bar{v}^2+\bar{v}b)$$

ordenando

$$p(\bar{v}^3+\bar{v}^2b-b\bar{v}^2+\bar{v}b^2)T^{1/2}+a(\bar{v}-b)=RT^{3/2}\bar{v}^2+RT^{3/2}\bar{v}b$$

$$pT^{1/2}(\bar{v}^3+\bar{v}^2b-b\bar{v}^2+\bar{v}b^2)+a(\bar{v}-b)=RT^{3/2}\bar{v}^2+RT^{3/2}\bar{v}b$$

dividiendo

$$\frac{pT^{1/2}(\bar{v}^3+\bar{v}^2b-b\bar{v}^2-\bar{v}b^2)+a(\bar{v}-b)=RT^{3/2}\bar{v}^2+RT^{3/2}\bar{v}b}{pT^{1/2}}$$

$$\bar{v}^3+\cancel{\bar{v}^2b}-\cancel{b\bar{v}^2}-\bar{v}b^2+\frac{a(\bar{v}-b)}{pT^{1/2}}=\frac{RT\bar{v}^2}{p}+\frac{RT}{p}(\bar{v}b)$$

$$\bar{v}^3 - \bar{v}b^2 + \frac{a(\bar{v}-b)}{PT^{1/2}} = \frac{RT\bar{v}^2}{P} + \frac{RT}{P}(\bar{v}b)$$

ordenando términos

$$\bar{v}^3 - \bar{v}b^2 + \frac{a(\bar{v}-b)}{PT^{1/2}} - \frac{RT\bar{v}^2}{P} - \frac{RT}{P}(\bar{v}b) = 0$$

$$\bar{v}^3 - \bar{v}b^2 + \frac{a\bar{v}}{PT^{1/2}} - \frac{ab}{PT^{1/2}} - \frac{RT\bar{v}^2}{P} - \frac{RT}{P}\bar{v}b = 0$$

$$\bar{v}^3 - \frac{RT\bar{v}^2}{P} - \bar{v}b^2 + \frac{a\bar{v}}{PT^{1/2}} - \frac{RT}{P}\bar{v}b - \frac{ab}{PT^{1/2}} = 0$$

$$\bar{v}^3 - \bar{v}^2\left(\frac{RT}{P}\right) + \bar{v}\left(\frac{a}{PT^{1/2}} - \frac{RTb}{P} - b^2\right) - \frac{ab}{PT^{1/2}} = 0$$

Checando unidades

$$\bar{V}^3 - \bar{V}^2\left(\frac{RT}{P}\right) + \bar{V}\left(\frac{a}{PT^{1/2}} - \frac{RTb}{P} - b^2\right) - \frac{ab}{PT^{1/2}} = 0$$

$$\left(L/mol\right)^3 - \frac{L^2}{mol^2}\left(\frac{\frac{\cancel{atm}\,L}{mol\,\cancel{K}}\cancel{K}}{\cancel{atm}}\right) + \frac{L}{mol}\left[\frac{\cancel{atm}\,L^2/mol^2\,\cancel{K^{1/2}}}{\cancel{atm}\,\cancel{K^{1/2}}} - \frac{\frac{\cancel{atm}\,L}{mol\,\cancel{K}}\cancel{K}\;L/mol}{\cancel{atm}} - \left(\frac{L}{mol}\right)^2\right]$$

$$- \frac{\frac{\cancel{atm}\,L^2}{mol^2}\cancel{K^{1/2}}\;\frac{L}{mol}}{\cancel{atm}\,\cancel{K^{1/2}}} = \left(\frac{L}{mol}\right)^3 - \left(\frac{L}{mol}\right)^3 + \left(\frac{L}{mol}\right)^3 - \left(\frac{L}{mol}\right)^3$$

OK ✓

Tarea

Revisar Ec. Virial

Temp. Boyle

Factor de compresibilidad