Example question: Phase equilibrium - Solution

In a bottle composed of 490 mL water, 490 mL air, and 20 mL octanol, 42.1 mg of 1-hexene is spiked. Assuming that the bottle is a closed system and equilibrium partitioning is established for 1-hexene, determine the mass of 1-hexene partitioned in each phase (in mg) and the 1-hexene fugacity (in atm) value in the bottle. (50 points)

Answer)

For 1-hexene,

$H_{pc} = 10^{2.55}\ atm-L/mole,\ \ K_{ow} = 10^{3.40}$

Calculate Z values:

$$Z_{air} = \frac{1}{RT} = \frac{1}{0.0821\ L-atm/mole-k \times 298\ K} = 0.0409\ mole/L-atm$$

(for any substance at 25℃ 1 atm, $Z_{air} = 0.0409\ mole/L-atm$)

$$Z_{water} = \frac{1}{H_{pc}} = \frac{1}{10^{2.55}\ atm-L/mole} = 2.82 \times 10^{-3}\ mole/L-atm$$

$$Z_{oct} = \frac{K_{ow}}{H_{pc}} = \frac{10^{3.40}}{10^{2.55}\ atm-L/mole} = 7.08\ mole/L-atm$$

Now, construct a table as below:

Phase	Volume (L)	Z_i (mole/L-atm)	$Z_i \times V_i$ (mole/atm)	$(Z_i \times V_i)/\Sigma(Z_i \times V_i)$	mass (mg)
Air	0.490	0.0409	0.0200	0.123	5.18
Water	0.490	0.00282	0.0138	0.00847	0.36
Octanol	0.020	7.08	0.143	0.801	36.67
		$\Sigma(Z_i \times V_i)$ =	0.163		

Note $mass_i = mass_{total} \times \{Z_i V_i / \sum(Z_i V_i)\},\ \ mass_{total} = 42.1\ mg$

What is the fugacity value?

$$mass_{total} = f_i \times \sum (Z_i V_i)$$

$$f_i = \frac{mass_{total}}{\sum (Z_i V_i)} = \frac{0.0421\ g}{0.163\ mole/atm} = 3.07 \times 10^{-3}\ atm$$