Calculating Isoprene in Liquid Phase

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Sean Weise 8-20-12

Using Henry's Constant for Determining the Amount of Isoprene in the Liquid Phase

Things you need to know

1. The amount of isoprene in the gas phase (mols)
2. The total pressure of the gas phase, usually assumed to be atmospheric pressure 101,000 (Pa)
3. Volume of the liquid phase

Math

Amount of isoprene in gas phase (mols) ÷ Volume of gas phase (L) * [1]25 (L mol^{-1}) * [2]101,000 (Pa) ÷ [3]H_{pc} (Pa L mol^{-1}) * Volume of liquid phase (L) = Amount of isoprene in the liquid phase (mols)

Explanation

[1] This is the volume of 1 mole of an ideal gas at 25°C. By multiplying this you end up with a mole fraction of isoprene i.e. moles of isoprene / moles air
[2] This is the pressure of the gas phase, in most case we assume it to be atmospheric pressure which is 101 kPa or 101,000 Pa. By multiplying by this you end up a partial pressure of isoprene in the gas phase
[3] This is Henry's Constant. By dividing by this you end up with a molarity of isoprene in the liquid phase

Equation for Henry's Constant (H_{pc})

$H_{pc} = e^{(-(\Delta H/RT)+C)}$

H_{pc} = Henry's constant units $Pa_{isoprene}$ $L_{liquid\ volume}$ $mol^{-1}{}_{isoprene\ in\ liquid}$
ΔH = enthalpy change of volatilization which we estimated to be **39100 J mol^{-1}** by averaging data from other monoterpines (Copolovici and Niinemets, 2005)
R = ideal gas constant **8.314 J mol^{-1} K^{-1}**
T = temperature of liquid phase units °K (which is 273.1 + °C)
C = empirical constant which we determined to be **31.6434** given an H_{pc} of 7780000 Pa L mol^{-1} at 25°C (Copolovici and Niinemets, 2005)

Copolovici, L.O. and Niinemets, U. (2005) Temperature dependencies of Henry's law constants and octanol/water partition coefficients for key plant volatile monoterpenoids. *Chemosphere* **61**, 1390-1400.