Mathematical Development of Emulsion Flavor Release Model (Equation 1)

A flavor compound that is in an oil and water mixture and in a closed system with air will equilibrate and distribute itself between these mixture phases and air in a constant ratio, at a given temperature. The flavor mass is redistributed in these different phases according to the different partition coefficients.

$m_I = m_A + m_W + m_O$; Emulsion case (mixture with an oil volumic fraction f_o) (1)

$m_I = m_A + m_W$; Water case (1b)

$$K_{AW} = \frac{C_A}{C_W} \qquad K_{OW} = \frac{C_O}{C_W} \qquad (2)$$

with m referring to the flavor mass at equilibrium, K referring to partition coefficient and C referring to flavor concentration. The subscripts $_I$, $_A$, $_W$ and $_O$ refer respectively to Initial, Air, Water and Oil .

As a first hypothesis in the model, we disregard any irreversible ab- or adsorption between flavor compounds and any mixture component such as lactose or milk protein. We set that each flavor compound F with an initial mass m_I, has only three possible environments to distribute: air, water and oil phases. All non-lipid phases in the samples are counted as "water".

Experimentally, we followed the headspace peak area released in air after equilibration for the emulsion case: $(m_A)_{fo}$, flavor mass in the air phase for a system with a oil volumic fraction f_O, normalized to the headspace peak area of the same flavor compound released in water: $(m_A)_{water}$. This measured amount is the expression (3).

$$\frac{(m_A)_{fo}}{(m_A)_{water}} \qquad (3)$$

Replacing m_A by its value from expression (1),

$$\left(\frac{m_A}{m_I}\right)_{fo} = 1 - \frac{m_O + m_W}{m_I} = 1 - \frac{V_O C_O + V_W C_W}{V_A C_A + V_O C_O + V_W C_W} \qquad (4)$$

with V referring to the phase volume.

This later expression is then multiplied by the identity term of $(1/V_T C_A)/(1/V_T C_A)$. V_T refers to the mixture volume ($V_O + V_W$). Using the expression (2), we obtain:

$$\left(\frac{m_A}{m_I}\right)_{fo} = 1 - \frac{\frac{V_O}{V_T}\frac{C_O}{C_A} + \frac{V_W}{V_T}\frac{C_W}{C_A}}{\frac{V_A}{V_T}\frac{C_A}{C_A} + \frac{V_O}{V_T}\frac{C_O}{C_A} + \frac{V_W}{V_T}\frac{C_W}{C_A}} = 1 - \frac{f_O K_{OA} + (1 - f_O) K_{WA}}{\left(\frac{V_A}{V_T}\right)_{f_o} + f_O K_{OA} + (1 - f_O) K_{WA}} \qquad (5)$$

Because $K_{OA} = \frac{C_O}{C_A} = \frac{C_O}{C_W}\frac{C_W}{C_A} = K_{OW} K_{WA}$, Then (5) can be written as:

$$\left(\frac{m_A}{m_I}\right)_{fo} = 1 - \frac{K_{WA}(f_O K_{OW} + f_W)}{K_{WA}(f_O K_{OW} + f_W) + + \left(\frac{V_A}{V_T}\right)_{f_o}} \qquad (6)$$

We proceed in the same way for the water case by using the expression (1b).

$$\left(\frac{m_A}{m_I}\right)_{water} = \left(1 - \frac{m_W}{m_I}\right)_{water} = 1 - \frac{V_W C_W}{V_W C_W + V_A C_A}$$

multiplied by the identity term of $(1/V_W C_A)/(1/V_W C_A)$,

$$\left(\frac{m_A}{m_I}\right)_{water} = 1 - \frac{\frac{V_W}{V_W}\frac{C_W}{C_A}}{\frac{V_W}{V_W}\frac{C_W}{C_A} + \frac{V_A}{V_W}\frac{C_A}{C_A}} = 1 - \frac{K_{WA}}{K_{WA} + \left(\frac{V_A}{V_W}\right)_{water}}$$

Finally, we obtain:

$$\frac{(m_A)_{fo}}{(m_A)_{water}} = \frac{\left(\frac{m_A}{m_I}\right)_{fo}}{\left(\frac{m_A}{m_I}\right)_{water}} = \frac{1 - \frac{K_{WA}(f_O K_{OW} + f_W)}{K_{WA}(f_O K_{OW} + f_W) + \left(\frac{V_A}{V_T}\right)_{fo}}}{1 - \frac{K_{WA}}{K_{WA} + \left(\frac{V_A}{V_T}\right)_{water}}} = \frac{\left(\frac{V_A}{V_T}\right)_{fo}\left(K_{WA} + \left(\frac{V_A}{V_T}\right)_{water}\right)}{\left(\frac{V_A}{V_T}\right)_{water}\left(K_{WA}(f_O K_{OW} + f_W) + \left(\frac{V_A}{V_T}\right)_{water}\right)}$$

where f_w is the water volumic fraction ($f_w + f_o = 1$).

As the model is based on volumic fraction, the density of milkfat (0.86g/ml) was also taken into account. Each experiment was made in a 2ml vial.

In case of water, the mass of aqueous solution was 800mg, $V_A = V_{vial} - V_W$ was then 1.2ml .

In case of emulsions,

$$V_A + V_O + V_W = 2ml$$

$$f_O = \frac{V_O}{V_O + V_W}$$

$$d = 0.86 = \frac{m_{fat}}{V_O} \Rightarrow V_O = \frac{m_{fat}}{0.86}$$

$$V_T = V_O + V_W = \frac{V_O}{f_O} = \frac{m_{fat}}{0.86 f_O}$$

$$V_A = 2 - \frac{m_{fat}}{0.86 f_O}$$