APPENDIX A

1. Percent of relative standard deviation (% RSD)

Percent of relative standard deviation can be calculated from the following equation.[48]

$$\% \text{ RSD} = (\text{SD} / \overline{\text{X}}) * 100$$

Where

% RSD = percent of relative standard deviation

SD = standard deviation

$\overline{\text{X}}$ = mean measured value

SD can be calculated from the following equation :

$$SD = \sqrt{\sum_{i=1}^{n} \frac{(x_i - \overline{x})}{n-1}}$$

Where

x_i = individual measured

n = number of measurements

APPENDIX B

A definition of limit of detection (LOD) is based on the concentration, which gives a signal equals to the blank signal plus three standard deviation of the blank.[49-50] LOD is calculated from the calibration curve by means of the blank signal, which can be used as an estimation of the calculated intercept, plus three standard deviations of the blank. It can be used as an estimation of the calculated value from the regression line.

The limit of detection is calculated from the linear regression line of the calibration curve as :

$$y = bx + a \qquad (1)$$

where

y = instrument signals

x = concentrations

a = intercept

b = slope of the straight line

$$Y_L = Y_B + kS_B \qquad (2)$$

where

Y_L = lowest detectable instrument signals

Y_B = Blank signal

$Y_B \cong$ intercept, a

k = constant depending on definition such as k = 1.5, 3 or 10 according to IUPAC, in this work k = 3 is used.

S_B = blank signal standard deviation

$S_B \cong S_{y/x}$

$S_{y/x}$ can be calculated from the equation :

$$S_{y/x} = [\Sigma (Y_i - \hat{Y}_i)^2 / (n-2)]^{1/2} \quad (3)$$

where

Y_i = respondse value from the instrument corresponding to the individual x – values

$\hat{Y}_i$ = value of y on the calculated regression line corresponding the individual x – values

n = number of points on the calibration line

From equation (2) and (3)

$$Y_L = a + 3S_{y/x} \quad (4)$$

$$Y_L = a + bC_L$$

Thus, the concentration at detection at detection limit(C_L) can be calculated by using the equation(6)

$$a + 3S_{y/x} = a + bC_L \quad (5)$$

$$C_L = 3S_{y/x} / b \quad (6)$$

Calculation of limit of detection in term of the least amount of ethanol by using the data from Table B1. The linear regression equation is $y = 0.001x + 0.0003$.

Table B1 Calculation data of the concentration of ethanol on the linear regression equation.

Concentration(ppm)	Yi	$\hat{Y}_i$	$\lvert Y_i - \hat{Y}_i \rvert$	$\lvert Y_i - \hat{Y}_i \rvert^2$
10.00	0.0107	0.0103	0.0004	1.6×10^{-7}
20.00	0.0192	0.0203	0.0011	1.2×10^{-6}
40.00	0.0445	0.0403	0.0042	1.8×10^{-5}
60.00	0.0602	0.0603	0.0003	9.0×10^{-8}
			$\Sigma \lvert Y_i - \hat{Y}_i \rvert^2$	1.9×10^{-5}

$$S_{y/x} = [1.9 \times 10^{-5} / (4-2)]^{1/2}$$

$$= 3.1 \times 10^{-3}$$

$$C_L = 3S_{y/x} / b$$

$$C_L = (3 * 3.1 \times 10^{-3}) / 0.001$$

$$= 9.25 \text{ mg/L}$$

$\therefore$ LOD of ethanol = 9.25 mg/L

Characteristics of regression equation and calculated concentrations of acetone is shown in Table B2. The linear regression equation is $y = 0.0012x + 0.0028$.

Table B2 Calculation data of the concentration of acetone on the linear regression equation.

Concentration(ppm)	Yi	$\hat{Y}_i$	$\lvert Y_i - \hat{Y}_i \rvert$	$\lvert Y_i - \hat{Y}_i \rvert^2$
5.00	0.78	0.89	0.108	0.0118
10.00	1.49	1.50	0.008	0.0001
20.00	2.93	2.72	0.212	0.0448
40.00	5.07	5.16	0.088	0.0078
			$\Sigma \lvert Y_i - \hat{Y}_i \rvert^2$	0.0644

$$S_{y/x} = [\Sigma (Y_i - \hat{Y}_i)^2 / (n-2)]^{1/2}$$

$$S_{y/x} = [0.0644 / (4-2)]^{1/2}$$

$$= 0.180$$

$$C_L = 3S_{y/x} / b$$

$$C_L = (3*0.180) / 0.122$$

$$= 4.41 \text{ mg/L}$$

$\therefore$ LOD of acetone = 4.41 mg/L

VITAE

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