APPENDIX

1. Calculation of Detection Limit [52]

A commonly used definition of detection limit in the literature of analytical chemistry is the analyte concentration giving signal equal to the blank signal plus three standard deviations of the blank. In this work, the detection limit was calculated from the calibration curve by means of the blank signal, which can be used as an estimate of the calculated intercept, plus three standard deviations of the blank. It can be used as an estimate of the calculated value from the regression line.

detection limit was calculated from the Linear Least Squares' Line procedure.

$y = a + bx$ (1)
y = instrument signals
x = normally are concentrations
a = intercept
b = slope of the straight line
$Y_L = Y_B + k\,S_B$ (2)
Y_L = lowest detectable instrument signals
$Y_B \cong$ intercept, a
k = constant depending on definition such as $k = 3$, 1.5, or 10 According to IUPAC, in calculation of detection limit, $k = 3$ was used and in this work this value was used.
S_B = blank signal standard deviation
$\cong S_{y/x}$

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

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

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

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

n = number (of points) on the calibration line

From equation (2) and (3)

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

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

$$Y_L = a + b\,C_L$$

Thus

$$a + 3\,S_{y/x} = a + b\,C_L$$

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

Example from the data of the calibration curve of nitrate with the concentration range 0.06-0.6 ppm.

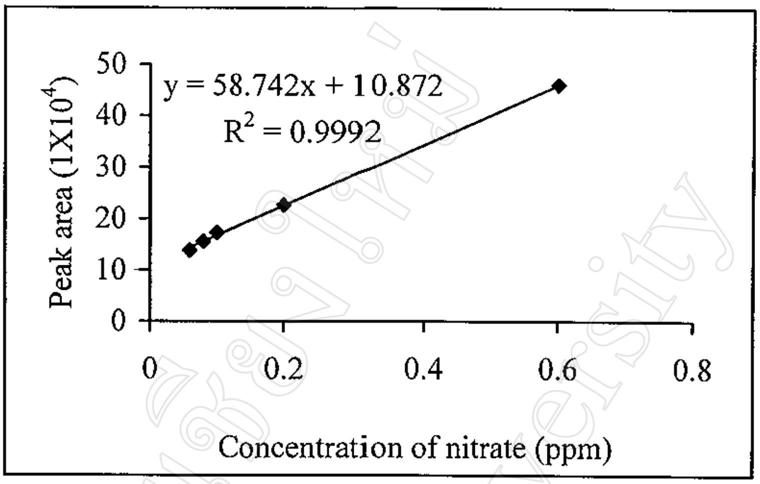

Figure A-1 Calibration curve of nitrate.

Concentration (ppm)	Y_i	$\hat{Y}_i$	$[Y_i-\hat{Y}_i]$	$[Y_i-\hat{Y}_i]^2$
0.06	13.864	14.396	0.532	2.830×10^{-1}
0.08	15.568	15.571	0.003	9.000×10^{-3}
0.10	17.282	16.746	0.536	2.870×10^{-1}
0.20	22.675	22.620	0.055	3.025×10^{-3}
0.60	46.064	46.117	0.053	2.809×10^{-3}
			$\Sigma [Y_i-\hat{Y}_i]^2$	0.576

$$S_{y/x} = [0.576/(5-2)]^{1/2}$$

$$= 0.438$$

$$C_L = (3 \times 0.438) / 58.742$$

$$= 0.022 \text{ ppm}$$

$\therefore$ Detection limit $\cong$ 0.022 ppm

2. Reproducibility of results [53]

Precision of analysis may be defined as the concordance of a series of measurements of the same quantity. The number of measurements required will depend on the accuracy required and on the known reproducibility of the method. The precision can be expressed as the standard deviation (S.D) and the relative standard deviation (% R.S.D). The smaller the value of the relative standard deviation and the relative standard deviation are defined by equations (1) and (2), respectively.

$$\text{S.D} = \sqrt{(X_i-\bar{X})^2/(n-1)} \qquad (1)$$

$$\%\,\text{R.S.D} = (\text{S.D}/\bar{X})\,100 \qquad (2)$$

where X_i = the individual value in data
$\bar{X}$ = the mean of data
N = the number of measurement

3. Percent recovery of anions in water samples

Percent recovery of each anion in water samples was qualitatively confirmed using the "spike" method, with the addition of known amount of standard solution of each anion to water samples at various concentrations.

Calculation for the % recovery was made via the following relationship.

$$\%\,\text{Recovery} = (A-B)\,100/C$$

where A = the amount of anion in natural water sample obtained with standard solution spiked at various concentrations

B = the amount of anion in natural water sample obtained without spiking anion solution

C = concentration of standard anion solution spiked to natural water sample

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