Appendix

To calculate the uncertainties of y (MAT) (σ_y):

$$\sigma_y^2 = \boldsymbol{AMA^T}$$

where

$$\boldsymbol{A} = \begin{bmatrix} \frac{\partial y}{\partial a} & \frac{\partial y}{\partial b} & \frac{\partial y}{\partial x} \end{bmatrix}$$

and

$$\boldsymbol{M} = \begin{bmatrix} \sigma_a^2 & cov_{ab} & 0 \\ cov_{ab} & \sigma_b^2 & 0 \\ 0 & 0 & \sigma_x^2 \end{bmatrix}$$

, i.e. **M** is the variance-covariance matrix, and $\mathbf{A}^{\mathbf{T}}$ is transpose of matrix **A**.

$$\sigma_y = \sqrt{\left(\frac{\partial y}{\partial a}\right)^2 \sigma_a^2 + \left(\frac{\partial y}{\partial b}\right)^2 \sigma_b^2 + \left(\frac{\partial y}{\partial x}\right)^2 \sigma_x^2 + 2\frac{\partial y}{\partial a}\frac{\partial y}{\partial b} cov_{ab}} = \sqrt{x^2\sigma_a^2 + \sigma_b^2 + a^2\sigma_x^2 + 2x\rho_{ab}\sigma_a\sigma_b}$$

From this, we can calculate the confidence and prediction bands by using

$$\sigma_{y_{CI\,95\%}} = t_{(1-\frac{\propto}{2},n-2)}\sigma_y$$

and

$$\sigma_{y_{PI\,95\%}} = t_{(1-\frac{\propto}{2},n-2)}\sqrt{\sigma_y^2 + \sigma_0^2}$$

, where t is the t score equal to N-2 degrees of freedom from the Student's distribution, α=1-(confidence level/100) (confidence level is 95% here), and σ_0 (RMSE of the regression) is

$$\sigma_0 = \sqrt{\frac{\sum_{k=1}^{N}\left(\left(y_i - y_p\right)^2\right)_k}{N-2}}$$

, where N is the number of independent x_i-y_i data pairs for regression, y_i is the original MAT data and y_p is the predicted y (i.e. predicted MAT values using the regression model).