Appendix

To calculate the uncertainties of $y$ (MAT) ($\sigma_y$):

$$\sigma_y^2 = A M A^T$$

where

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

and

$$M = \begin{bmatrix} \sigma_a^2 & \text{cov}_{ab} & 0 \\ \text{cov}_{ab} & \sigma_b^2 & 0 \\ 0 & 0 & \sigma_x^2 \end{bmatrix}$$

, i.e. $M$ is the variance-covariance matrix, and $A^T$ is transpose of matrix $A$.

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

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

$$\sigma_{yCL\_95\%} = t_{(1-\frac{\alpha}{2},n-2)}\sigma_y$$

and

$$\sigma_{yFL\_95\%} = t_{(1-\frac{\alpha}{2},n-2)}\sqrt{\sigma_y^2 + \sigma_0^2}$$

, where $t$ is the $t$ score equal to N-2 degrees of freedom from the Student’s distribution, $\alpha$=1- (confidence level/100) (confidence level is 95% here), and $\sigma_0$ (RMSE of the regression) is

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

, 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).