

## Statistics for the OTC model evaluation

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The statistical formulations presented in each spreadsheet are as follows:  $P_i$  and  $O_i$  are the individual (daily maximum or average, depending on the parameter) predicted and observed concentrations, respectively;  $\bar{P}$  and  $\bar{O}$  are the average concentrations, respectively; and  $N$  is the sample size.

(1) Coefficient of determination,  $R^2$ :

$$R^2 = \frac{\left[ \sum (P_i - \bar{P})(O_i - \bar{O}) \right]^2}{\sum (P_i - \bar{P})^2 \sum (O_i - \bar{O})^2}$$

(2) Normalized mean error, in %:

$$NME = \frac{\sum |P_i - O_i|}{\sum O_i} \times 100\%$$

(3) Root mean square error, in ppb or  $\mu\text{g m}^{-3}$ :

$$RMSE = \left[ \frac{1}{N} \sum (P_i - O_i)^2 \right]^{1/2}$$

(4) Fractional gross error, in %:

$$FE = \frac{2}{N} \sum \left| \frac{P_i - O_i}{P_i + O_i} \right| \times 100\%$$

(5) Mean absolute gross error, in ppb or  $\mu\text{g m}^{-3}$ :

$$MAGE = \frac{1}{N} \sum |P_i - O_i|$$

(6) Mean normalized gross error, in %:

$$MNGE = \frac{1}{N} \sum \frac{|P_i - O_i|}{O_i} \times 100\%$$

(7) Mean bias, in ppb or  $\mu\text{g m}^{-3}$ :

$$MB = \frac{1}{N} \sum (P_i - O_i)$$

(8) Mean normalized bias, in %:

$$MNB = \frac{1}{N} \sum \frac{(P_i - O_i)}{O_i} \times 100\%$$

(9) Mean fractionalized bias, in %:

$$MFB = \frac{2}{N} \sum \left[ \frac{P_i - O_i}{P_i + O_i} \right] \times 100\%$$

(10) Normalized mean bias, in %:

$$NMB = \frac{\sum (P_i - O_i)}{\sum O_i} \times 100\%$$