Log-Linear Plots for Data Representation

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When developing models to represent experimental data, residual plots are effective for assessing quality of fit, and these present the differences between data and reference data or a model. However, when some ordinate values are excessive, it is impossible to maintain definition for small values. This happens when highly accurate and precise data are compared to much less accurate and/or precise data. It is customary to present two plots: one for near zero ordinate values and one for high ordinate magnitudes. We present a plotting method which covers the entire ordinate range on a single plot with adequate definition in all regions.

Plotting Arrangement and Transformation

Display of both small and large residual values on a single axis requires using two plots or a "broken" scale. It is possible to include all values on a single axis which uses a combination of logarithmic and linear scales and is compatible with commercial plotting packages. If we define the ordinate such that tick marks on the linear scale are common to some of those on the logarithmic scale, the procedure can use commercial packages because it requires only a single linear scale with specific labels for the ordinate.

A transformation which satisfies these constraints for a set of data $\{(y_i, x_i)\}$ results from plotting the ordinate values at locations given by:

$$
\begin{aligned}
y_i^* &= \left\{ y_c \left(\frac{y_i}{|y_i|} \right) \log_{10} \left| \frac{10 y_i}{y_c} \right| \right\} && \text{for } |y_i| > y_c \\
y_i^* &= y_i && \text{for } |y_i| \le y_c
\end{aligned}
\tag{1}
$$

where y_i^* is the transformed ordinate for plotting on a linear grid and y_c is the crossover value of y (that is, the maximum value for the linear portion of the plot or the minimum value for the logarithmic portion of the plot). Major divisions on the ordinate appear at integer multiples of y_c. The values for these major divisions are:

$$0, \pm y_c, \pm 10 y_c, \ldots, \pm 10^{n-1} y_c$$

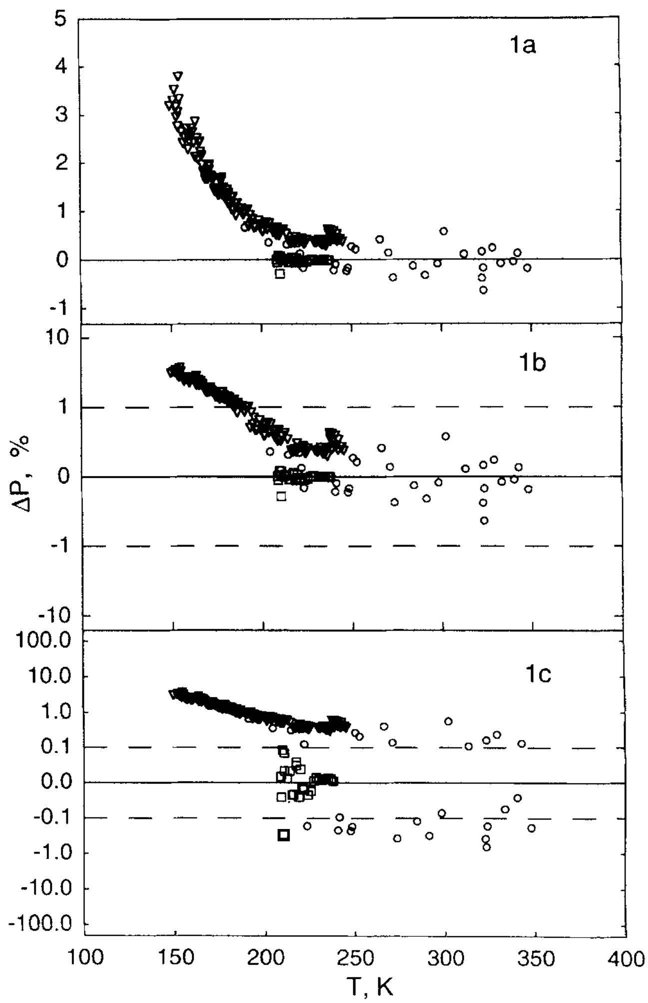

Figure 1. Vapor pressure deviation using: (a) normal linear plot; (b) log-linear scale with 0–1.0% linear; (c) log-linear scale with 0–0.1% linear.
∇ (Kanungo et al., 1987); ○ (Malbrunot et al., 1968); (Weber and Goodwin, 1993).

where n is the number of divisions removed from the zero value. The most convenient choices for y_c, are 0.1, 1, 10, and so on. We can also place minor division marks along the ordinate, such as at $\pm 0.5 y_c$, $\pm 3.16 y_c$, ..., $\pm 3.16(10^{n-1}) y_c$.

Example

Malbrunot et al. (1967), Kanungo et al. (1987), and Weber and Goodwin (1993) have published experimental values for the vapor pressure of difluoromethane (R-32). One of these sets of data has high accuracy and precision, one set is of moderate accuracy, and one set is significantly different from the other two. We examine the deviations from a model proposed by Weber and Goodwin (1993):

$$\ln P = n_1 + \frac{T_C}{T}(n_2\tau + n_3\tau^{1.5} + n_4\tau^{2.5} + n_5\tau^5) \qquad (2)$$

with $T_C = 351.36$, $n_1 = 8.666202$, $n_2 = -7.42533$, $n_3 = 1.57051$, $n_4 = -1.64501$ and $n_5 = -3.39793$. Figure 1a is a conventional linear plot. The large discrepancies of the Malbrunot et al. (1967) data dominate the plot and mask the details of the deviations for the other two sets. Figure 1b is a log-linear plot with $y_c = 1.0\%$. This plot provides ample definition for the older data and for the intermediate set, but it presents a somewhat restricted view of the best data. Figure 1c is a log-linear plot with $y_c = 0.1\%$ which contains ample detail for the best data, but retains information about the other two sets. The method provides a convenient way to illustrate consistency, or lack therefore, among different data sets.

Conclusions

We have proposed a method to plot values that range from small to large on a single plot without losing definition of structure for the small values. This plotting procedure is convenient when using commercial software, because it consists of a transformation of the data which enables them to be plotted on a linear scale with differently labeled divisions.

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