Solution to precision mixology challenge

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The winner of the precision mixology challenge (published in volume 408, issue 1) is:

Sami T. Tuomivaara, Complex Carbohydrate Research Center, University of Georgia, Athens, GA, USA

The award entitles the winner to select a Springer book of his choice up to a value of €100,-.

Our Congratulations!

Solution

Alice has a three-decimal-digit digital balance, which can weigh up to 100 g [1]. If she performs a single six-fold dilution of the stock solution with the mass fraction of cadmium $w_0 = 3000 \mu\text{g/g}$, then the following equation can be written for the mass fraction of cadmium in the final solution, w_{Cd} :

$$w_{Cd} = w_0 \frac{m_{\text{aliquot}}}{m_{\text{final}}} \quad (1)$$

where $m_{\text{aliquot}} \approx m_{\text{final}}/6$. Best results are always obtained when m_{final} is as large as possible, i.e., 100 g in this case. The uncertainty of w_{Cd} is estimated via uncertainty propagation as follows:

$$\frac{u^2(w_{Cd})}{w_{Cd}^2} = \frac{u^2(m_{\text{aliquot}})}{m_{\text{aliquot}}^2} + \frac{u^2(m_{\text{final}})}{m_{\text{final}}^2} \quad (2)$$

$$\frac{u^2(w_{Cd})}{w_{Cd}^2} = \frac{0.002^2}{100.0^2/6^2} + \frac{0.002^2}{100.0^2} = 0.00012^2 \quad (3)$$

If Alice performs serial dilution of the stock solution n -times, each time diluting the stock k_i times where $i = 1, 2, \dots, n$ and $k_1 \times k_2 \times \dots \times k_n = K = 6$, then the following equation can be written for the mass fraction of cadmium in the final solution, w_{Cd} :

$$w_{Cd} = w_0 \frac{m_{1,\text{aliquot}}}{m_{1,\text{final}}} \times \frac{m_{2,\text{aliquot}}}{m_{2,\text{final}}} \times \dots \times \frac{m_{n,\text{aliquot}}}{m_{n,\text{final}}} \quad (4)$$

The relative uncertainty of w_{Cd} from Eq. 4 can be evaluated similar as it was done for Eq. 1. For n -step dilution,

$$\frac{u^2(w_{Cd})}{w_{Cd}^2} = \sum_{i=1}^n \frac{u^2(m_{i,\text{aliquot}})}{m_{i,\text{final}}^2/k_i^2} + \sum_{i=1}^n \frac{u^2(m_{i,\text{final}})}{m_{i,\text{final}}^2} \quad (5)$$

Note that $m_{i,\text{final}} = (100 \pm 0.002) \text{ g}$ and $m_{i,\text{aliquot}} = (100 \pm 0.002)/k_i \text{ g}$. Given that all mass uncertainties are equal,

$$\frac{u^2(w_{Cd})}{w_{Cd}^2} = \frac{u^2(m)}{m_{\text{final}}^2} \sum_{i=1}^n (1 + k_i^2) \propto \sum_{i=1}^n (1 + k_i^2) \quad (6)$$

The best results are those with lowest relative uncertainty of w_{Cd} and we can find out what values of n and k_i in Eq. 6 satisfy this requirement. In other words, we are seeking the minimum value for $\sum_{i=1}^n (1 + k_i^2)$ as a function of n and k_i given the constrain $k_1 \times k_2 \times \dots \times k_n = K$. This condition is met when all dilution factors are equal, which means $k_i = \sqrt[n]{K}$. It remains now to find the optimal number of steps for serial dilution in order to achieve the desired dilution factor and guarantee the lowest relative uncertainty of w_{Cd} . This amounts to finding the minimum for function $\sum_{i=1}^n (1 + \sqrt[n]{K^2}) = n + n\sqrt[n]{K^2}$, which occurs at $n = 2.8 \approx 3$ for $K = 6$. The minimum at $n \approx 3$ is also shown in Fig. 1.

The best strategy for Alice is to serially dilute the 3000 $\mu\text{g/g}$ cadmium solution three times, each time using a

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Fig. 1 Uncertainty of w_{Cd} when serial dilution of 3000 $\mu\text{g/g}$ solution is performed in n steps, each time with a dilution factor of $k_i = \sqrt[n]{6}$ ($i = 1, 2, \dots, n$)

dilution factor of $\sqrt[3]{6}$. In this problem we have looked only at the mathematical side of the problem and one has to acknowledge other sources of errors in dilutions. For example, while a three-step serial dilution might be preferable from a mathematical point of view, each step can lead to potential contaminations from glassware and pipettes.

References

1. Meija J. *Anal Bioanal Chem.* 2016;408:7.