



A New Approach to Calculating the Non-exchangeable 2H Isotopic Composition of Hair and the Procedural Fractionation Factor by Treating the Molar Exchange Fraction as a Process Related Variable.

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Hair is a keratinous tissue that incorporates hydrogen from material that a mammal consumes but is metabolically inert following synthesis. The stable hydrogen isotope composition of hair has been used to track the migration of animals as well as for forensic and archaeological purposes to determine the provenance of human remains or geographic trajectories of living people. Only the non-exchangeable hydrogen in a hair sample ($\delta^{2}\text{HN}$) is metabolically informative but it cannot be measured directly. It is usually obtained by estimation using a commonly applied mathematical expression incorporating sample measurements obtained from two isotopically distinct equilibration procedures. This commonly used approach treats the fraction of exchangeable hydrogen as a mixing ratio, with the procedural fractionation factor (α_{P}) assumed to be close or equal to 1. Instead, we have used the full molar ratios to derive an expression for $\delta^{2}\text{HN}$ explicitly as a function of both the molar hydrogen exchange fraction (FEX) and α_{P} . A longitudinal study of a hair sample, using two isotopically distinct equilibration procedures and a process of iteration on α_{P} to determine $\delta^{2}\text{HN}$, demonstrates that FEX should be treated as a process dependent parameter, i.e. a reaction specific constant, just as α_{P} is. From a practical point of view it is not always possible to carry out such a longitudinal study to determine $\delta^{2}\text{HN}$, FEX and α_{P} . Consequently, two additional suggestions are made for future approaches for direct estimation of α_{P} . The first entails employing three rather than two isotopically distinct equilibrations. The second anticipates the future availability of standard hair material for isotopic analysis but suggests a novel use of this material.