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Closure in Concentration Data: Comparing the Magnitude of Material Transfer with System Size Change

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Closure poses interpretive challenges when evaluating compositional data because it forces component concentrations to sum to unity. This mathematical dependency contributes spurious variability to concentrations beyond those caused by material transfer. Fortunately, measuring the magnitude of closure's spurious variability is possible using the definition of a concentration: $\boldsymbol{x = X/S}$, where $\boldsymbol{x}$ and $\boldsymbol{X}$ represent a component's intensive concentration and extensive amount in a system, and $\boldsymbol{S}$ represents the size of the system. By taking this equation's derivative, dividing both sides by $\boldsymbol{x}$, and simplifying the result, we obtain a fundamental equation: $\boldsymbol{dx/x = dX/X - dS/S}$, demonstrating that the relative variability of a component concentration ($\boldsymbol{dx/x}$) is a function of the relative variability of the component's amounts ($\boldsymbol{dX/X}$) and the relative variability of the system size ($\boldsymbol{dS/S}$). Clearly, $\boldsymbol{dX/X}$ describes the relative amount of material transfer that took place. Thus, $\boldsymbol{dS/S}$ must be the amount of closure affecting the system's concentrations. Substituting a conserved component ($\boldsymbol{Z}$), where $\boldsymbol{dZ = 0}$, for $\boldsymbol{X}$ in our fundamental equation yields: $\boldsymbol{dz/z = -dS/S}$, so we must conclude that $\boldsymbol{dS/S}$ is a measure of the amount of closure, as $\boldsymbol{Z}$ undergoes no material transfer. Moreover, closure is a function of the relative size of the system, so its effect is the same for every component. Alternatively, examining concentrations of component ($\boldsymbol{Y}$) that were affected by material transfer ($\boldsymbol{dY \neq 0}$), we can also measure the relative amount of material transfer that took place ($\boldsymbol{dY/Y}$). Substituting the amount of closure ($\boldsymbol{dS/S = -dz/z}$) into our fundamental equation in $\boldsymbol{Y}$ and simplifying, we obtain: $\boldsymbol{dY/Y = dy/y - dz/z}$, and can now compare the magnitudes of closure and material transfer in compositional systems. Examples comparing the magnitudes of closure ($\boldsymbol{dS/S}$) and material transfer ($\boldsymbol{dY/Y}$) are presented using lithogeochemical data from a suite of New Zealand mudstones that exhibit very large and very small material transfers.