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ABSTRACT:

An Approximate Formulation of Multicomponent Diffusion Matrices for Silicate Melts and Glasses

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Ionic transport in silicate glasses and melts are at the core of many applications in material sciences and geosciences. Traditionally in the geosciences and increasingly in material sciences, the compositions of interest are multicomponent. Determination of the full diffusion coefficient matrix in such n-component systems typically require at least (n-1), and often more, diffusion couple experiments. This rapidly becomes prohibitively expensive in time and cost.
Therefore, it is of interest to develop approaches that allow approximate calculations of such matrices in order to provide at least first order estimates of coupled transport behavior, and to identify conditions at which experimental efforts could be focused. We suggest here a three step approach toward this goal. First, consideration of the universality of glass transition and relaxation behavior in silicate melts provides a connection between diffusivity and viscosity. The approach is different from merely using a Stokes-Einstein or Eyring kind of relationship to relate viscosity and diffusivity, which have been attempted in the past. Second, empirical models are now available for the calculation of viscosities with considerable accuracy for a wide range of melt compositions. Making use of these it is possible to predict the tracer diffusivity of ions of different charges with some degree of uncertainty. Finally, models to connect the tracer diffusivities to the elements of the multicomponent diffusion matrix may be used to calculate the full matrices. For this stage, several available models may be tested and refined with the help of available experimental data. This approach ensures that the eigenvalues and eigenvectors of the calculated matrices conform to the expected theoretical behaviors. It will be shown that this provides a pathway for calculating diffusion coefficient matrices, and exploring the nature of diffusive coupling, for arbitrary melt compositions. Such matrices are useful for the evaluation of thermal vs. chemical buoyancy effects during the mixing of melts of different compositions.