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Separating the effects of molecular mobility and miscibility on particle phase diffusion using the Maxwell-Stefan diffusion model

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Models of diffusion through organic particles can indicate whether the kinetic limitation imposed by viscous particles on gas-particle partitioning has a significant effect on aerosol transformation - an area of intense research. However, all concerned studies to date have used the Fickian framework for diffusion modelling and this is not generally applicable to non-ideal systems. Here we review the limitation of the Fickian framework for diffusion modelling and show how the Maxwell-Stefan approach is preferential. The latter framework does allow a generally applicable model through separating the effects of non-ideality (and therefore solubility) and molecular mobility on diffusion. Through a combination of molecular diffusivity estimates and activity coefficient estimates, the Maxwell-Stefan framework therefore offers the most robust approach to particle phase diffusion modelling. The model has been tested under a range of scenarios for changes to the saturation ratios of organic components and water and for multicomponent systems, with key results shown here. In addition to particle size and molecular mobility, the Maxwell-Stefan framework offers evaluation of gas-particle partitioning limitation as a function of component activity coefficients also. Model estimates of the partitioning fraction of semi-volatile components are thus presented under a range of molecular diffusivities and both positive and negative deviations from ideality.