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Inferring Chemical Kinetics from Direct and Indirect Concentration Data

Many chemical compounds used in the agricultural industry bring large amounts of arsenic into the soil. As this poses serious environmental hazards, designing safe and effective arsenic decontaminating agents is an active research area. To do this, it is crucial to understand chemical kinetics between arsenic and various geochemicals at the molecular level. However, state-of-the-art direct measurement techniques aggregate concentration measures making it impossible to infer individual reaction rates. Here we include the modelling of mass spectrometry data which serve as indirect proxies to individual chemical concentrations. The study ultimately seeks identifiability of parameters through simulated and real spectral data.