

A study of the aqueous phase equilibria involving the Fe(VI) species

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Ferrates (VI) are powerful oxidizing agents both in acidic and basic solutions; treatment of all kind of water sources collected worldwide have demonstrated their capability of removing a wide range of organic and inorganic compounds. Additionally, during the oxidation process, the $[\text{FeO}_4]^{2-}$ anions reacting with water lead to the *in situ* formation of Fe oxyhydroxide nanoparticles, which serve as an efficient adsorbent for oxidized pollutants and suspended/colloidal materials. However, these findings have not yet fully exploited to practical applications due to difficulties associated with the relatively low production yield and the limited stability field, as a function of pH, T, concentration and co-existing ions. Results of kinetic studies have shown the complexity of ferrates (VI) decay in aqueous solutions, with the formation of both oxygen and hydrogen peroxide together with a plethora of short-living intermediates. Despite the deeper knowledge-grade recently achieved, the results are not fully consistent, lacking a proper up-to-date overview on the relative thermodynamics and stability in water. Using PHREEQC, this study critically reviews the aqueous phase-equilibria of ferrate and the related aqueous species/complexes over the whole pH range through a specific updated Pourbaix diagram, focused on the stability region for the high-valent iron compounds. Results point out that the standard $[\text{FeO}_4]^{2-}$ stability field is further reduced while accounting for the presence of $\text{Fe}(\text{OH})_4^-$ [1], which is slightly more stable than $\text{Fe}(\text{OH})_3$. An additional new factor considered in regards to the previous studies is the O_2 partial pressure which, once increased to 1 atm, seems to extend the stability/predominance field of ferrate species. A set of laboratory experiments will follow in order to validate the computational results.

[1] Diakonov (1999) *Geochim. Cosmochim. Ac.* **63**, 2247-2261