

Simulation on the distribution of metal-picolinate complexes in the model waste solution

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Abstract

The distribution of vanadium and iron ionic species in the presence of picolinate ligand has been simulated and evaluated at different pH values and various compositions of the model waste solution. A computer program was useful for the calculation of the speciation of metal picolinate complexes. In spite of the variations of metal concentration, there are little differences in the shape of distribution diagrams under the high-picolinate LOMI condition if the molar ratio of picolinate to metal is fixed at a constant value. Also, for a model solution under low-picolinate LOMI condition, it is hard to find out some significant changes in shape of distribution diagrams regardless of the variations of metal concentration in solution. However, the reduced amount of picolinate from 6 times to 3 times on the basis of vanadium concentration affects shape of distribution diagrams. For vanadium(III)-picolinate complexes, a peak corresponding to the vanadium tris picolinate, $V(\text{Pic})_3$ is reduced greatly. In case of iron(II)-picolinate complexes, shape of the distribution diagram was changed significantly. In a model solution of low-picolinate LOMI condition, the fraction of iron(II) complex species is maintained at a constant ratio in the region over pH 4. Especially, the speciation of iron(II)-picolinate complexes is dependent upon the concentration of iron in a model solution under the low-picolinate LOMI condition. This phenomenon is attributed to the shortage of picolinate ligand in solution, and originated from the difference of stability constants between vanadium(III) and iron(II) species with picolinate