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PROPERTY DATA PREDICTION FOR HAZARDOUS SUBSTANCES

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Abstract

Results are presented for property data prediction of hazardous substances. Predictive constants (group contribution, interaction parameter and structural correction values) are disclosed to predict critical constants of temperature, pressure and volume. The model using the disclosed values is applicable to a wide variety of substances cited as hazardous by RCRA (Resource Conservation and Recovery Act). The wide variety of substances includes hydrocarbons, alcohols, acids, ketones, aldehydes, ethers, epoxides, esters, amines, nitriles, sulfides, thiols, fluorides, chlorides, bromides and iodides.

Testing of the model yielded favorable findings for prediction of critical constants. For critical temperature, testing with over four hundred substances produced an average absolute deviation between observed and predicted values of only 0.63%. For critical pressure, testing with over two hundred and ninety substances indicated an average absolute deviation of 2.53%. For critical volume, an average absolute deviation of 1.42% was experienced in testing with over two hundred substances.

SOLIDIFICATION OF HAZARDOUS SUBSTANCES – A TGA AND FTIR STUDY OF PORTLAND CEMENT CONTAINING METAL NITRATES

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Abstract

Type I Portland cement samples containing the soluble nitrates of the priority pollutant metals chromium, lead, barium, mercury, cadmium and zinc have

been investigated by using thermogravimetric and fourier-transform infrared techniques (including diffuse reflectance). The major vibrational bands and thermal stability of the carbonate, sulfate, silicate, water and nitrate species are tabulated and discussed in comparison to uncontaminated Portland cement. The solubility and volatility of mercury in cement and the effect of metal nitrate concentration on the silicate condensation process is discussed. Although results suggest that retardation of cement setting by Zn and Pb salts occurs by limiting hydration, the chemistry of the two processes is distinctly different.

SURFACE INVESTIGATIONS OF THE BINDINGS OF METALS IN CONCRETE

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Abstract

The chemical nature of solidified hazardous waste is an important consideration for modeling the stability and the design of appropriate systems. This study uses X-ray photoelectron spectroscopy, XPS, ion scattering spectroscopy, (ISS) and electron microscopy (qualitative and analytical) to examine the chemical nature of metal ion doped Portland cement. Chromium, lead, cadmium, mercury and zinc systems have been examined as to the morphology of the cement and the nature of the binding of these metals. These surface studies are beginning to delineate the mutual effects of the pollutants and the containment system. A model for the retardation of cement settings by lead has been developed and the chemical nature of Hg in cement has been determined. These developments are presented along with similar observations and results on the other metals.