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