Calculating service life time for compound chemicals with group contribution compensation

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Traditionally, cartridge service life time prediction for organic contaminants is based on the Wood equilibrium model, an empirical adsorption equilibrium formulation correlated from a large database of test data. While this approach works for most OV chemicals, those chemicals with special functional groups, such as the amino group, may exhibit large deviation from the actual data. In this research, we use a group contribution method to amend the Wood model calculation. We test the service life of the target cartridge with simple chemical containing the functional group of interest. The group contribution of this functional group is extracted by comparing the test results with those predicted by the Wood model. This special group contribution is applied to any other chemicals containing this special functional group to offset the calculation deviation. To validate this theory, we select the amino group (NHx) as our subject. We correlate the adsorption equilibrium data for ammonia and methyl amine from test data. The equilibrium data is then compared with the Wood model prediction, and the group contribution of the amino group is extracted from the differences. This group contribution is then used to compensate the Wood model for some other amino derivatives. Comparison of the compensated results with the test data show that the group contribution approach can greatly decrease the service life calculation error from the traditional Wood model.