

Risk-Based Prioritization Scheme for Hazardous Waste Chemicals Using Modeled Exposure and Toxicity Estimate

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The objective of this project was to develop a ranking scheme for screening and prioritizing large groups of chemicals based on modeled estimates of toxicity and exposure. This method was applied to approximately 220 Hazardous Waste Identification Rule (HWIR) chemicals, most of which lacked experimental toxicity data. Commercial Quantitative Structure Activity Relationship (QSAR) models were used to estimate the noncancer toxicity potential of the chemicals, while CALTOX 4.0 was used to estimate the exposure potential of the HWIR chemicals. A relative Hazard Quotient (rHQ) was then determined using the modeled toxicity and exposure estimate. The chemical ranking was achieved by using a Classification and Regression Tree (CART) approach that grouped chemicals based on similarities in their exposure and toxicity potentials. The CART algorithm is a nonparametric statistical procedure that classifies data via a series of “yes/no” questions concerning the physicochemical properties of chemicals. Initially, chemicals with similar exposure potentials were assigned, based on their physicochemical properties, into groups or “bins.” The average exposure of the chemicals in a given group was then chosen to represent the exposure potential of all of the chemicals in that group since this procedure would reduce the number of steps in the ranking process. The HWIR chemicals were then grouped in increasing order of hazard potential based on their modeled or estimated values of exposure and toxicity. In summary, this method uses both modeled exposure and modeled toxicity estimates to develop a relative ranking based on overall noncancer risk. It offers a more consistent and comparative approach than previous risk-based methods, using a variety of exposure and toxicity models, and can be applied to various chemical groups, such as the Candidate Contaminant List (CCL). We hope now to establish contacts and work with program and regional offices of solid waste, water, and toxics to validate and make greater use of this approach and to assist in prioritizing and addressing the most important chemical risks facing our society.