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Analytics in Chemical Process Investigations

Dr. John Fildes was an expert in a case involving exposure to chemicals used in water treatment, which also provides insight to investigation of other chemical processes. The opposing side sought to settle this case after Dr. Fildes had submitted his report, even before he was deposed.

Water treatment is a process in which various chemical are added to effect desired chemical transformations and other chemicals are produced as a result. Several water treatment processes exist, and their chemical transformations are well established. The chemical composition of the source water can vary substantially, making water treatment a challenging chemical process to investigate.

The individual who claimed exposure to the products of the water treatment process had collected samples that were chemically analyzed, which was the basis for their exposure claim. Dr. Fildes was retained as an expert by the defendant. His work covered the sample collection and chemical analyses obtained by the opposing side, chemical analyses of the water treatment process conducted by an independent authority, analysis of the water treatment process and source water chemistry, and testing to establish the properties of the material produced by the water treatment process and of its ability to be transported to remote locations. Dr. Fildes is able to handle the wide range of issues that arise in complex and multidisciplinary technical issues because he had a broad and fundamental experience with the scientific issues that underlie chemical processes and materials.

Two chemical analyses were obtained by the opposing side and were claimed to prove that an individual was exposed to the products of a water treatment process. The analysis identified about 20 chemical species and the concentrations of these chemical species differed in the two samples as is typically the case. The concentrations of the chemical species in the two samples also each differed from their concentrations in existing chemical analyses of the products of the water treatment process. Nonetheless, an engineer used by the opposing side concluded that the collected samples were similar to the analyses of the products of the water treatment process, thereby establishing exposure to the products of the water treatment process in his opinion. This situation is not unusual in chemical process investigations, which often involve assessing the concentrations of many chemical species that can vary substantially from sample to sample. This type of investigation therefore calls for use of analytics rather than simply eyeballing the data and using arbitrary judgement of what constitutes a meaningful difference.

Applying Analytics – Data Mining

The products of a chemical process sometimes provide a fingerprint of the process because the concentrations of the chemical species in the products of the process are related to each other through the chemical equations for the transformations that occur. This suggests that the similarity of samples can be objectively established by either computing statistical tolerance intervals if enough data exists, or by treating the concentrations of each of the chemical species as components of vectors (one vector for each sample) and using cluster analysis to probe their similarity. In this case, Dr. Fildes computed statistical tolerance intervals, but he has also used cluster analysis in other situations. A tolerance interval is a statistical interval that uses the mean concentration and standard deviation of each chemical species to estimate a concentration interval for each chemical species that could occur by chance. A commonly used interval is one for which there is 95% confidence the interval would contain 95% of the measured concentrations if a large number of samples had been measured. Confidence intervals overlap for similar samples.

Cluster analysis establishes the similarity of samples by using the concentrations of each species as components of vectors and identifying if the vectors lie in approximately the same direction in space and have about the same magnitude. To understand this, suppose that different people start at the same place and walk different directions and different distances, each person ending at a point specified by its x and y coordinates. The x and y coordinates are the components of a vector and there would be a vector for each person. Cluster analysis would establish which vectors reside in the same region of space.

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Applying Analytics – Chemical Process Modeling

Data mining will typically have limits to the insight it can produce because the data that exists is typically limited in the number of samples that exist and may have been collected far in the past, which can be addressed by modeling the chemical process using the chemical equations for the transformations that occur. In water treatment, several chemical reactions occur to differing degrees depending on the chemical composition of the source water, which varies substantially. Modeling involved using the measured chemical concentrations of the species in the source water as input to the chemical equations describing the chemical transformations that took place during the process to predict the chemical composition of the products of the process. This provided predictions on a day by day basis for a one year periods, which allowed (1) an objective, quantitative assessment of how the chemical composition varied by year and of the uncertainty that should be expected in measured data, (2) estimation of how the chemical composition would vary throughout the storage area, and (3) validation of if the chemical composition from samples that came from portions of the storage area were representative of the entire storage area. Chemical process modeling was the only way to investigate this incident because it had occurred years in the past and the source water composition and products of the water treatment process vary over the years and seasons of each year.

The Daubert decision requirement for the admissibility of scientific evidence emphasized that science is a process rather than a static body of knowledge, and that to qualify as scientific knowledge an inference or assertion must be derived by the scientific method, which is described as a validation technique, involving the formulation of hypotheses and either experiments or observations to test the validity of them. (Imwinkelried, Edward J. (1993) "The Daubert Decision on the Admissibility of Scientific Evidence: The Supreme Court Chooses the Right Piece for All the Evidentiary Puzzles," Journal of Civil Rights and Economic Development: Vol. 9: 1, Article 2). Combining data mining with modeling based on available properties and scientific principles embodies the validation process at the heart of the Daubert decision and provides a compelling way to meet the rules of evidence.

The cause and origin of accidents and failures involving complex and multidisciplinary issues usually cut across the underlying disciplines and thus require a multidisciplinary perspective and use of analytics. Combining data mining and analytics to arrive at a conclusion by different independent means provides a compelling outcome that is easy for anyone to understand even if they do not understand the specifics of each of the analysis methods. This is why Dr. Fildes was able to provide a comprehensive, compelling report in a case with complex issues, with the outcome being that the opposing party initiated settlement discussions and the case settle without Dr. Fildes even being deposed.

Dr. John Fildes has a Ph.D. in physical chemistry, a B.S. in chemistry, and he was a post-doctoral research associate in a chemical engineering department. Physical chemistry provides the scientific basis for many engineering disciplines. Thermodynamics provides the basis for metallurgy, materials science, fire and explosion science, and others. Chemical bonding provides the basis for the strength of materials and electronic materials and devices. Electrochemistry provides the basis for corrosion science, and chemical kinetics provides the basis for chemical compatibility, reactivity, volatility, and chemical processes. Dr. Fildes has conducted over $27.5 million of R&D and/or litigation-related investigations in these areas because he is well experienced in the fundamental scientific principles as well as in analytics and chemical safety. He led a large group of scientists and engineers at Northwestern University and two scientific/engineering firms licensed to practice professional and structural engineering that conducted thousands of litigation-related technical investigations, so he is also an expert in the conduct of these types of investigations.