

David E. Simon, Ph.D., DES Consulting Bartlesville, OK

DESConsulting@sbcglobal.net

David completed his Ph.D. at IowaStateUniversity in 1972, studying both the geochemistry of calcite to dolomite conversion of limestone and highway concrete aging. After graduation, he became an exploration geologist for Texaco, Inc. gaining experience in the petroleum industry. He studied the effects of well completion fluids on gas and oil bearing formations as a research scientist for Halliburton Energy Services at their research center in Duncan, Oklahoma. David has published papers concerning geochemistry and material science using x-ray diffraction and awarded numerous patents for his contributions to the petroleum industry. He has spent more than 20 years developing Rietveld modeling techniques for the petroleum industry including the first complete refinement method for Portland cement using selective extractions. Since 2001, he has been involved in applying Rietveld Refinement to x-ray diffraction data at ConocoPhillips Research Center X-ray Technology Laboratory. His research included catalyst materials, scale samples from production facilities, geologic samples and high temperature in-situ studies of catalysts. After retirement in 2012, David has consulted with industry (petroleum industry, manufacturing, and mining), instrument vendors, software developers, and academic institutions focusing on the application and optimization of Rietveld refinement using "Phase Filters".

He will present the following paper:

PHASE FILTER ANALYSIS OF MATERIALS – THE NEW X-RAY DIFFRACTION TECHNOLOGY

Rietveld refinement analysis of x-ray diffraction patterns of samples has been evolving over the past 40 years. However, classic practice has been to perform search/match analysis of each sample using the preconceived biases of the scientist to limit the search/match results. Following this, the scientist develops the Rietveld refinement input file of the phases identified for each individual sample.

Refinement results are then compared to the actual data and further search/match performed to account for additional phases to explain the remaining peaks in the residual. This methodology can consume large amounts of time for each sample at high overhead costs.

The Rietveld refinement method using a "phase filters" is a concept where a small structure library of possible compounds could greatly simplify complex x-ray diffraction patterns. The input file in the model is designed to include a large number of possible phases that may or may not be present in the pattern. The refinement process allows the x-ray scientist to focus on interpreting the phases not identified by the "phase filter". A Rietveld refinement "phase filter" is designed to be able to:

- have 25+ unique phases in the input file,
- set the relative ratio of each line to a value of I_{max} greater than 0.0,
- set the scale factor to 0.0 whenever the factor becomes negative for an individual phase, and
- constrain the peak profile to instrumental values based on a reference standard, i.e. NIST 660.

Rietveld refinement with "phase filters" helps to improve the quality of interpretations, as well as, the consistency of x-ray diffraction results between laboratories and produce results in a very timely manner.