

APPLICATIONS OF PCFPW FUNDAMENTAL PARAMETERS SOFTWARE IN CORPORATE R&D AND QUALITY CONTROL ANALYTICAL LABORATORIES

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Fundamental parameters software has evolved considerably since the theoretical basis for these programs was developed in the 1970's and early 1980's and the advent of the personal computer. Fundamental parameter theory takes into account any possible interelement interactions by using a series of known physical parameters, such as mass absorption coefficients, x-ray fluorescence yields, jump ratios, transition probabilities, etc. These parameters along with instrument conditions, an estimate of sample composition, and at least one standard per element (not necessarily in the same matrix) are used in an iterative process to calculate sample concentrations.

Approximately five years ago Fundex Software and Technology, Inc., on behalf of the Dow Chemical Company, began development of a software program called PCFPW or Personal Computer Fundamental Parameters for Windows. This software uses the NIST algorithm to model the x-ray tube spectrum and an improved algorithm for computing mass absorption coefficients. This improved algorithm reflects the most recent mass absorption coefficient data in the literature. The software user-interface was developed in collaboration with XRF specialists at the Dow Chemical Company to meet the needs both of a corporate R&D analytical laboratory serving a variety of functions and manufacturing quality control laboratories.

This software has been used extensively at the Dow Chemical Company for the last three years at eleven different sites worldwide. This paper will illustrate how this software is used to meet the fast-paced needs of research and industrial support. Specific examples will be presented that demonstrate the wide spread applicability of this software program including polymer analysis, adhesives, latex, epoxy and brine.