TOF Profile function used at POWGEN:

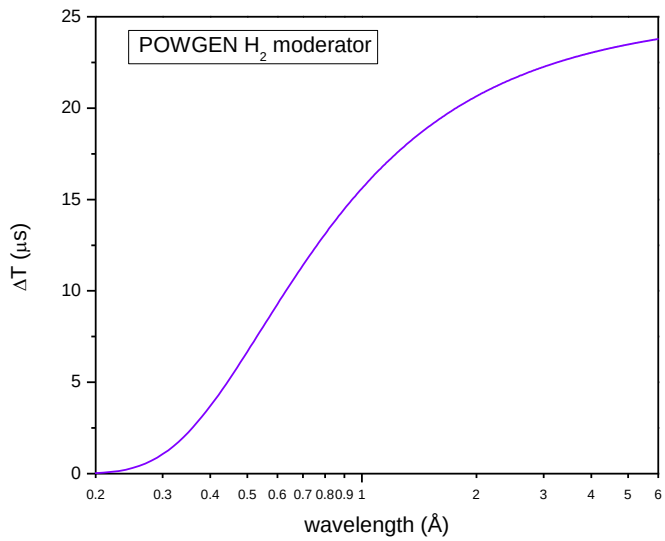
Powgen uses a TOF profile function which is a variation on the standard profile function originally derived by VonDreele, Jorgensen and Windsor (VonDreele RB, Jorgensen JD and Windsor CG, "Rietveld Refinement with Spallation Neutron Powder Diffraction Data", *J. Appl. Cryst.* **15**, 581 (1982). This function is implemented in GSAS (profile function 3, 4 & 5) and Fullprof NPROF 9 and is most applicable to diffractometers viewing ambient polyethylene or water moderators.

The POWGEN diffractometer, however, views a poisoned cryogenic H_2(liquid) moderator. The variation in peak shape and peak position with TOF (or d-spacing d) is calculated using a more complex function related to thermal and epithermal components of the neutron spectrum that was worked out by J.P. Hodges (unpublished) by fitting experimental data at GPPD and is now used for calibration of POWGEN diffraction patterns.

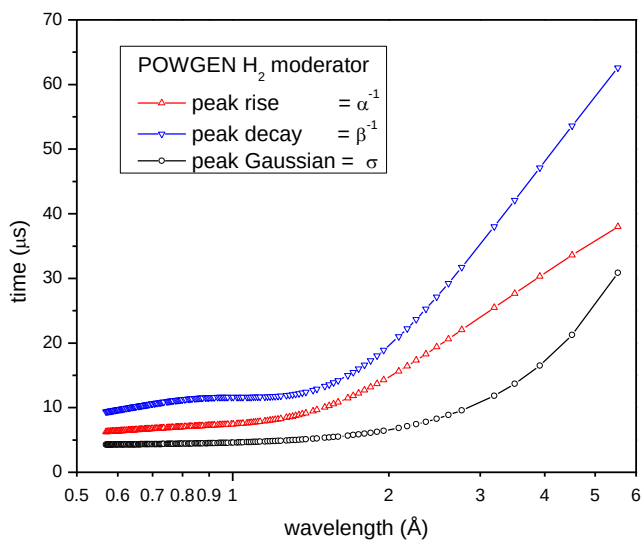
While the Rietveld program Fullprof (NPROF 10) and Jana implements the dependencies using the complex analytical expression proposed by Hodges (Fullprof users see following pdf for description), GSAS uses a lookup table incorporated in the parameter files that are available on the instrument webpage. The profile function are termed as -3,-4,-5 have peak shape broadening as described for the original profile functions 3, 4 & 5 in GSAS (manual describes 3, 4 and 5 in pages 147-155). However, the -3,-4,-5 profile functions use a table of α and β coefficients along with a correction to the reflection position in place of the regular GSAS d-spacing dependences. This method is referred to in the GSAS manual as been appropriate way to handle the complex behavior of cryogenic moderators. The two major components that differ are the d to TOF and the back-to-back exponentials α and β

- In profile function 3 (4 & 5), the d to TOF conversion is calculated using the following
  - $T = DIFC*d + DIFA*d^2 + Zero$
  - However in function -3,
    $T = DIFC*d + DIFA*d^2 + Zero + \Delta T$
    where ΔT is the deviation from the prior equation, and is recorded as one of the columns in the instrument parameter file tables.
    In some cases, it may be required to refine DIFA which provides some correction for sample displacement. The moderator emission time effect is completely taken care of by the table which is generated from calibration measurements of a NIST standard.

- The graph below shows how ΔT behaves as a function of wavelength for the POWGEN moderator:



- In profile function 3 (4 & 5), the values of the exponential α_1/d are described by the following
  - $\alpha = \alpha_1/d$ and $\beta = \beta_0 + \beta_1/d^4$
  - Again in function -3, the values of α and β are stated as a function of d spacing in the instrument parameter file tables.
  - The graph below shows how the underlying peak shape parameters (rise time, decay time and Gaussian width) vary as a function of wavelength for the POWGEN moderator:



- To summarize; the parameter file includes a table (for each profile #) that lists
    - d spacing, ΔT, α and β.
    - To see how these tabulated values are calculated refer to the Fullprof TOF manual.
- Apart from T, α and β, the other profile parameters are treated in the same manner as in profile function 3 (4 & 5).
- For the pseudo-Voight width parameters, we generally find the biggest contribution comes from sigma-2 and gamma-1. We use a default value of 10 for sigma-1 as this is the minimum GSAS currently allows. Our NIST calibration standards indicate a smaller value for sigma-1. User samples, however, may possess real peak broadening due to microscopic strains that increases sigma-1 > 10. When this is the case sigma-1 can also be refined to model the observed peak widths.