

Details of Misc/Capillary_Transmission

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Short Description: Provides X-ray transmission through a capillary tube mounted in a holder with a circular window.

Parameters	Description
x	Independent variable in the form of a scalar or an array
Xh	center of the hole in mm if the capillary is mounted within a hole
Dh	width of hole in mm if the capillary is mounted within a hole
Xch	Center of the capillary tube w.r.t the hole center
Dc	Inner diameter of the capillary tube in mm
tc	thickness of glass wall in mm
lc	absorption length of capillary tube wall in mm
ls	absorption length of sample inside the capillary tube
Db	width of the X-ray beam in mm assuming the beam profile to rectangular
norm	Normalization factor
bkg	background
Npt	No. of points to be used for beam profile convolution

Details: The Capillary Transmission function calculates the ratio of the intensities of the transmitted X-rays to the incident X-rays as a function of the position, x , of a capillary tube, holding a sample within it, with respect to the direct X-ray beam. The absorption lengths of the capillary tube and the sample are assumed to l_c and l_s , respectively. The capillary tube of inner diameter, D_c , and thickness, t_c , is assumed to be placed on a capillary tube holder with a circular window as shown in Figure 1. The hole is assumed to be centered at X_h from the direct beam position along the X-direction, and the capillary tube is assumed to be offset by X_{ch} from the hole center.

$$T(x) = \exp \left(-2 \left(\frac{t_{sx}(x, D_c, X_c, X_{ch})}{l_s} + \frac{t_{cx}(x, D_c, X_{ch}, t_c, D_h) - t_{sx}(x, D_c, X_c, X_{ch})}{l_c} \right) \right) H(x, D_h, X_h)$$

Where,

$$t_{sx} = \sqrt{\left(\frac{D_c^2}{4} - (x - X_h + X_{ch})^2 \right)} \quad \forall \quad |x - X_h + X_{ch}| \leq \frac{D_c}{2}$$
$$= 0 \quad \forall \quad |x - X_h + X_{ch}| > \frac{D_c}{2},$$

$$t_{cx}(x, D_c, X_{ch}, t_c, D_h, X_h) = \sqrt{\left(\frac{(D_c + 2t_c)^2}{4} - (x - X_h + X_{ch})^2\right)} \forall |x - X_c + X_{ch}| \leq \frac{D_c + 2t_c}{2}$$

$$= 0 \forall |x - X_c + X_{ch}| > \frac{D_c + 2t_c}{2},$$

and

$$H(x, D_h, X_h) = 0 \forall |x - X_h| > \frac{D_h}{2}$$

$$= 1 \forall |x - X_h| \leq \frac{D_h}{2}$$

The above function is only for X-ray beams of point size. For the X-ray beam of finite size the above function needs to be convoluted with the square function, $B(x, D_B)$, where D_B is the beam width. Hence, the transmission function, broadened by the beam finite beam width with an arbitrary normalization, $norm$, and background, bg , can provided by:

$$T_B(x) = norm * T(x) \otimes B(x, D_B) + bg$$

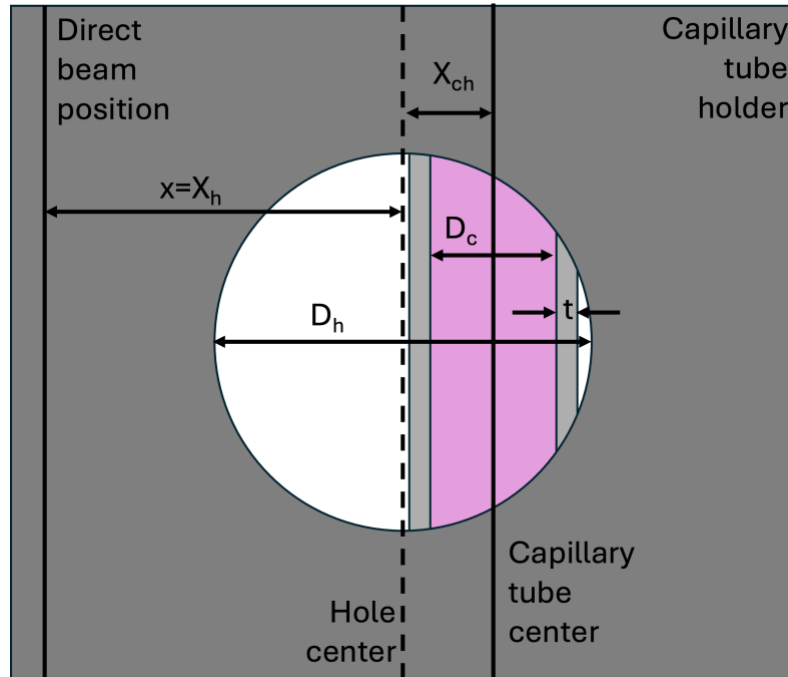


Figure 1 Schematics of the front view of the capillary tube within a capillary tube holder

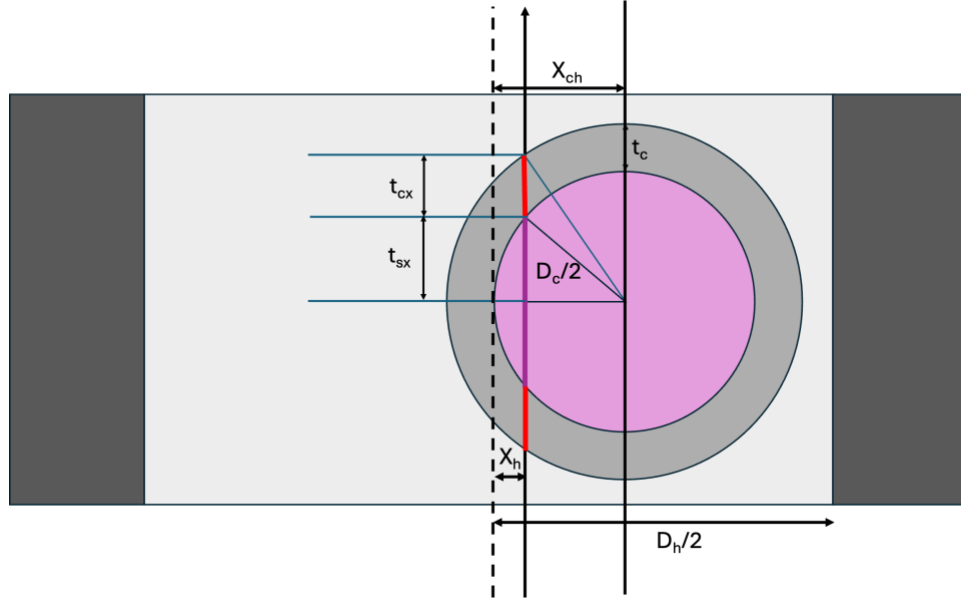


Figure 2: Schematics of the top view of the capillary tube within a capillary tube holder to show different transmission regions when the direct beam transmits through the capillary tube.

It is noted that while trying to fit the function with experimental transmission data collected from capillary tubes mounted on a capillary tube holder with circular window, the Levenberg-Marquardt algorithm does not fit the hole parameters, X_h and D_h . The global minimization algorithm provided by 'Differential-Evolution' can only be used to obtain the optimized X_h and D_h parameters along with other parameters. The issue with global optimization is it does not provide error-bars on the parameters. Hence, error-bars on other parameters can be obtained by again carrying out the fit with the Levenberg-Marquardt algorithm and fixing the hole parameters to the values obtained from global optimization.

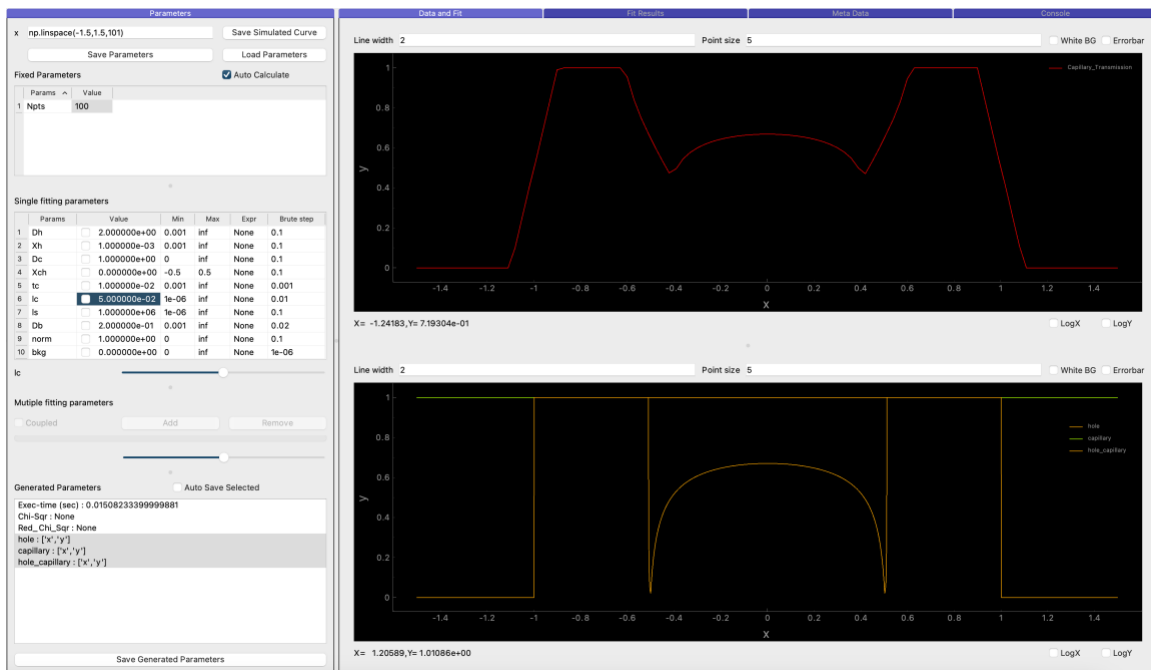


Figure 3 Screenshot of parameters and plots of the function