Self-shielding and single and double scattering calculations for scattering systems with cylindrical/annular geometry

Introduction

This application calculates "self-shielding" ("self-absorption") factors for an N-component "scattering system" comprising a central cylinder and N-1 concentric annuli. In the most trivial case N=1 and the system is a simple cylinder. Systems with N=2 are the hollow cylinder and the filled cylinder, and examples of systems with N=4 are shown in fig. 1. The integrals required for these calculations are performed in equal steps or using one of two variants of the Monte Carlo method, in which case double scattering intensities are also calculated (in the isotropic scattering approximation). The application handles situations where the beam does not fully illuminate the scattering system and it allows for an optional oscillating radial collimator (ORC).

A "typical" (actually atypical) setup is shown in fig. 2. Incident neutrons travel in the +x direction, the (x,y) scattering plane is normal to the axis of the scattering system, and the scattering system is centered at the origin. The incident beam is assumed to be uniform, monodirectional and centered at $y=\Delta$, $z=\Delta_z$. Its half-width and half-height are W and H respectively. The radius of the central cylinder is R_1 and the outer radii of successive annuli are R_2, R_3, etc, such that $R_1< R_2< R_3\ldots$ The height of the scattering system is H_0. The macroscopic scattering, absorption and total removal cross sections for region k are $\Sigma_{S,k}$, $\Sigma_{A,k}$ and $\Sigma_{T,k}=\Sigma_{S,k}+\Sigma_{A,k}$ respectively. These cross sections are assumed to remain unchanged on scattering. (This is certainly true to the extent that the scattering is elastic.)

An ORC, if present, is characterized by the angular separation between adjacent blades, 2α, the blade thickness 2δ, and its inner and outer radii, r_1 and r_2 respectively (fig. 3).

Usage

To use this application go to "Tools|General Tools|Miscellaneous|Self-shielding, cylindrical/annular geometry".

(1) Click on the "Examine/edit sample information" button and enter an appropriate problem description. Edit the number of regions and hit <CR>. As

necessary, edit the information for each region. Notice that two cross sections are required for each region. For self-shielding and single scattering calculations all that matters is the sum, but for double scattering calculations separate scattering and absorption cross sections are required. Remember to hit <CR> after each data entry. Click "Done" when you're done. You may wish to click again on the "Examine/edit sample information" button to confirm that the information has been accepted as expected.

(2) In the "Incident beam dimensions" box enter the beam width 2W, beam height 2H, and displacements Δ and Δ_z.

(3) In the "Oscillating Radial Collimator" box check "YES" if you want to include an oscillating radial collimator in the calculation. You may then edit the collimator parameters 2α, r_1, r_2 and 2δ (see above), and/or the (x,y) location of the collimator axis; the default values apply to the DCS oscillating radial collimator.

(4) In the "Start, stop and step …" box enter the lowest and highest scattering angles and the step in scattering angle.

(5) Under "Calculation Method" choose among numerical and two types of Monte Carlo (MC) calculations (see below). If it is to be a numerical calculation enter the number of integration steps. For a Monte Carlo calculation enter the number of steps and a positive integer seed; non-numerical entries and non-positive entries generate a random seed. Note that the time for an analytic calculation is roughly proportional to the square of the number of integration steps whereas for a Monte Carlo calculation it is directly proportional to the number of Monte Carlo steps. Numerical calculations only generate single scattering intensities whereas Monte Carlo calculations generate both single and double scattering intensities.

(6) To start the calculation hit "CALCULATE". Typically self-shielding factors are plotted. Individual or summed scattering fractions may be plotted by clicking on the appropriate button. For Monte Carlo calculations the ratio of double to single scattering may also be plotted. For further details see below.

The average transmission of the sample,

$$T_{average} = \frac{1}{2W}\int_{\Delta-W}^{\Delta+W} dy \exp\left\{-\sum_{k=1}^{N}\Sigma_{T,k}p_k(y)\right\},$$

where $p_k(y)$ is the distance through region k for neutrons with transverse coordinate y, as well as its transmission through a diameter,

$$T_{diameter} = \exp\left\{-\sum_{k=1}^{N}\Sigma_k p_k(\Delta)\right\} = \exp\left\{-2\sum_{k=1}^{N}\Sigma_k\left(R_k - R_{k-1}\right)\right\}$$

(with R_0=0) are displayed near the bottom left corner of the application window.

(7) To overplot the results of different calculations (e.g. numerical and Monte Carlo, or different samples), click the "Overplot" button. To perform a new calculation click the "New plot" button.

(8) The "File" menu allows you to save the results of a calculation, to display the sample geometry, to save or restore input parameters, to print the current plot to a postscript file, to view this help file, and to quit.

(9) The "Options" menu allows you to suppress or display plot legends, and to omit or show quantities that are zero at all scattering angles.

Results

To understand the results of the calculations consider the count-rate in a detector placed at scattering angle 2θ. The contribution due to single scattering within region K and subsequent escape to the detector may be written as follows:

$$I_K^{(1)}(2\theta) = \left(\phi_0 A_0\right)\cdot S_K^{(1)}(2\theta)\cdot\left(\Delta\Omega/4\pi\right)$$

where ϕ_0 is the incident "flux" (neutrons per unit area per unit time), A_0 is the area of the beam, $\Delta\Omega$ is the solid angle subtended by the detector, and

$$S_K^{(1)}(2\theta) = \left(\Sigma_{S,K}t_K^*\right)f_K(2\theta)$$

is the *single scattering fraction* for region K at scattering angle 2θ. In the latter expression

$$t_K^* = \frac{1}{2W}\int_{\Delta-W}^{\Delta+W} dy\, p_K(y) = V_K / A_0$$

is the effective thickness and

$$f_K(2\theta) = \frac{1}{V_K}\int_{V_K} d\mathbf{r} \exp\left\{-\sum_{k=1}^{N}\left[\Sigma_{T,k}d_k^{in}(\mathbf{r}) + \Sigma_{T,k}d_k^{out}(\mathbf{r},2\theta)\right]\right\} g(\mathbf{r},2\theta)$$

is the *self-shielding factor* for region K; V_K is the illuminated volume of region K, $d_k^{in}(\mathbf{r})$ is the distance through region k to the scattering point **r** (which is by definition within region K), $d_k^{out}(\mathbf{r}, 2\theta)$ is the distance through region k from the scattering point **r** in the direction 2θ, and the function $g(\mathbf{r},2\theta)$ is the transmission of the ORC; if there is no ORC, g=1.

In analogy with $I_K^{(1)}(2\theta)$, the contribution to the detector count-rate due to scattering within region K followed by scattering in region K' and escape to the detector, $I_{KK'}^{(2)}(2\theta)$, is defined by the expression

$$I_{KK'}^{(2)}(2\theta) = \left(\phi_0 A_0\right) \cdot S_{KK'}^{(2)}(2\theta) \cdot \left(\Delta\Omega/4\pi\right)$$

where $S_{KK'}^{(2)}(2\theta)$ is the *double scattering fraction*.

Summed single and double scattering fractions are then $S^{(1)}(2\theta) = \sum_K S_K^{(1)}(2\theta)$ and $S^{(2)}(2\theta) = \sum_{K,K'} S_{KK'}^{(2)}(2\theta)$ respectively, and the double-to-single *scattering ratio* is simply $\delta(2\theta) = S^{(2)}(2\theta) / S^{(1)}(2\theta)$.

Monte Carlo calculations

Two variants of the Monte Carlo method are available to the user. Given a neutron's location and direction, they differ in how the distance to the next scattering event is determined.

In method A, cumulative removal probabilities are used to determine a removal point and the neutron's statistical weight is multiplied by the product of the total removal probability and the scattering probability $\left(\Sigma_S / \Sigma_T\right)$ for the region where removal occurs.

In method B, cumulative scattering probabilities are used to determine the scattering point and the neutron's statistical weight is multiplied by the total scattering probability.

In principle the methods are equivalent. Depending on individual scattering and absorption cross sections one or the other may be the better choice. The user is advised to experiment with both approaches.

Questions?

Contact John Copley if you have questions, concerns or complaints.

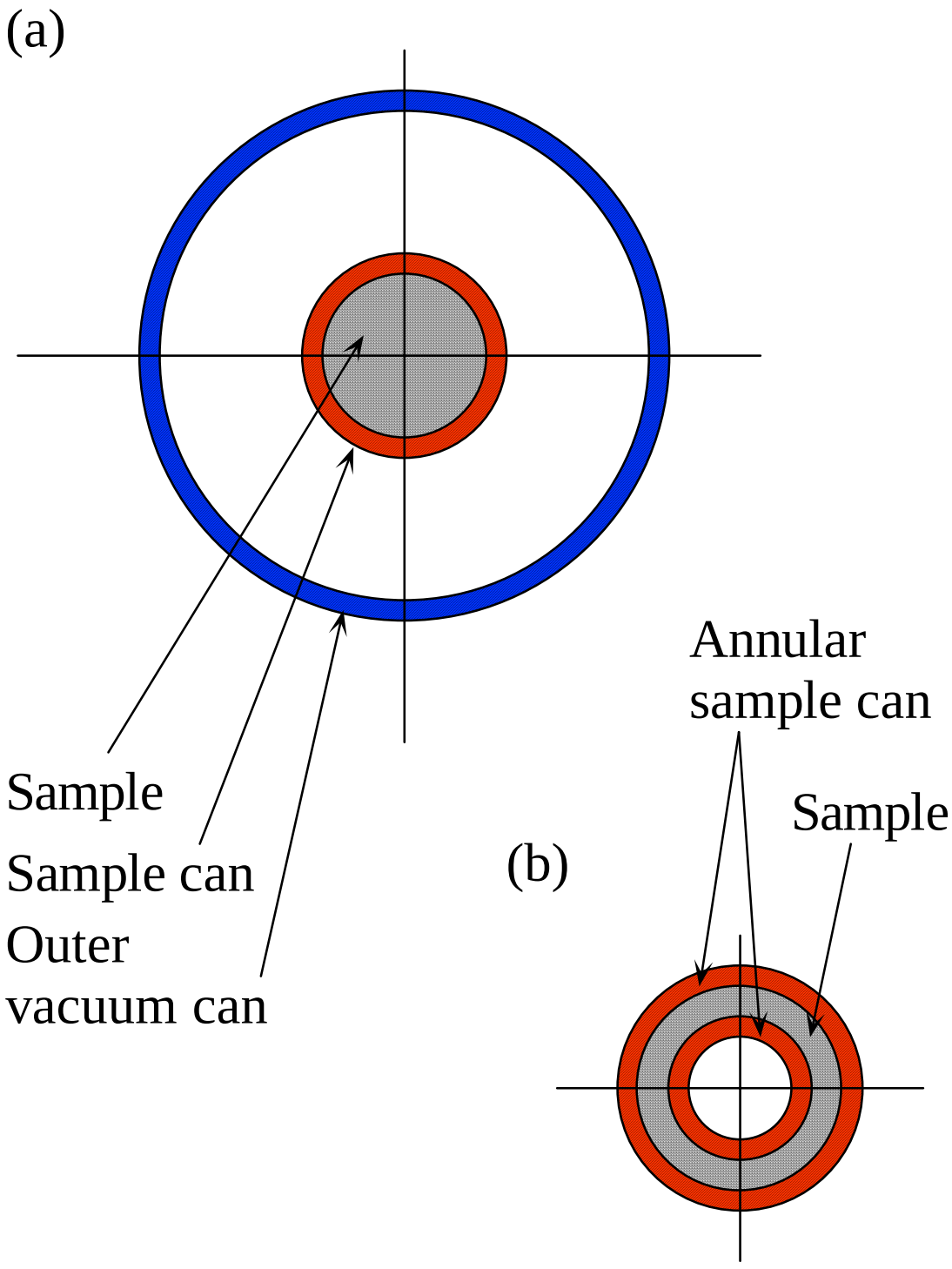
(a)
Sample
Sample can
Outer
vacuum can
(b)
Annular
sample can
Sample

Fig. 1

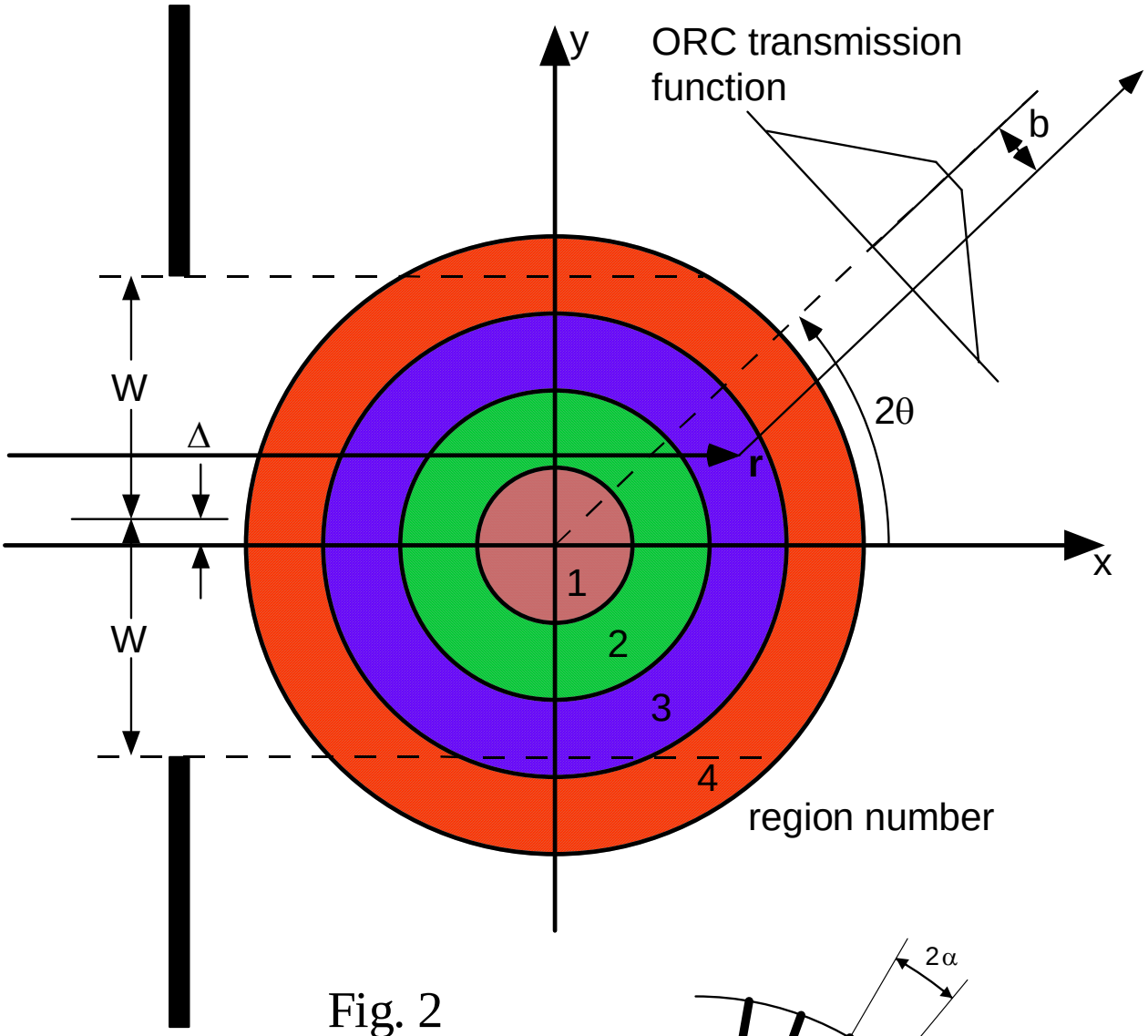
y
ORC transmission
function
b
W
Δ
2θ
r
x
1
2
3
4
W
region number

Fig. 2

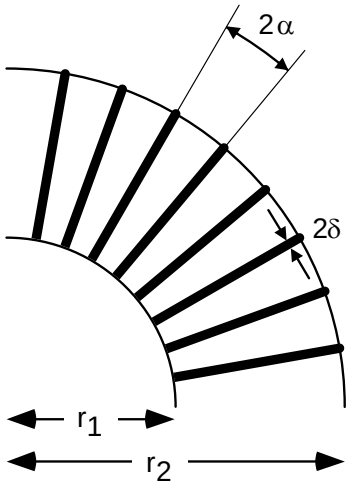
2α
2δ
r1
r2

Fig. 3