asc, an IDL program to calculate self-shielding factors

Introduction

The program *asc* ("Annulus Shielding Corrections") calculates so-called "self-shielding" ("self-absorption") factors for an N-component scattering system comprising a central cylinder and N-1 concentric annuli. In the simplest case N=1 and the system is a simple cylinder. Two examples of scattering systems with N=4 are shown in fig. 1. The program handles situations where the beam width is less than the diameter of the scattering system and/or the beam is not centered, and it accounts for the transmission properties of an (optional) oscillating radial collimator (ORC).

Theory

A "typical" (actually atypical) setup is shown in fig. 2. The calculation is in two dimensions, x and y. Incident neutrons travel in the +x direction, and the scattering system is centered at the origin. The incident beam is assumed to be uniform, monodirectional and centered at $y=\Delta$. Its half-width is W. 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 macroscopic removal cross section for region k, for neutrons of energy E, is $\Sigma_k(E)$.

The 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). Its transmission $g(\mathbf{r},2\theta)$ is a trapezoidal function (J.R.D. Copley and J.C. Cook, Nucl. Instr. Meth. A**345**, 313 (1994)):

$$g(\mathbf{r},2\theta) = t_0\left(1-\frac{\delta}{b_0}\right) \text{ if } |b| \le \delta; \quad t_0\left(1-\frac{|b|}{b_0}\right) \text{ if } \delta \le |b| \le b_0; \quad 0 \text{ if } b > b_0.$$

Here 2θ is the scattering angle, the scattering point is **r**, b is the impact parameter, i.e. the distance from **r** to a line from the origin in the direction 2θ (fig. 2), the maximum impact parameter b_0 is given by $b_0 = 2\alpha r_c - \left(\frac{1}{r_1}+\frac{1}{r_2}\right) r_c \delta$ with $\frac{1}{r_c} = \frac{1}{r_1} - \frac{1}{r_2}$, and the maximum transmission is $t_0 = \frac{b_0}{2\alpha r_c}$. It can be shown that $|b| = |x\sin 2\theta - y\cos 2\theta|$. If there is no ORC, g=1.

For a given measurement M the self-shielding factor for region K, $f_K^M(2\theta, E_i, E_f)$, is defined as follows:

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

where E_i and E_f are neutron energies before and after scattering, A_K is the illuminated area of region K in the x-y plane (e.g. the shaded area between the horizontal dashed lines in fig. 2), $d_k^{in}(\mathbf{r})$ 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 integral is performed over all points within the illuminated area A_K. The removal cross sections $\Sigma_k^{in} \equiv \Sigma_k(E_i)$ and $\Sigma_k^{out} \equiv \Sigma_k(E_f)$ depend on the experimental measurement (M).

For measurement M the neutron count rate may be written as follows:

$$I^M(2\theta, E_i, E_f) \approx C\sum_{K=1}^{N}\left[A_K \frac{d^2\Sigma}{d\Omega dE}(2\theta, E_i, E_f)\bigg|_K f_K^M(2\theta, E_i, E_f)\right]$$

with $C = \Phi \cdot \Delta\Omega(2\theta) \cdot h$, where Φ is the incident neutron flux (current density), $\Delta\Omega(2\theta)$ is the solid angle subtended by the detector at scattering angle 2θ and h is the illuminated height of the sample; $\frac{d^2\Sigma}{d\Omega dE}(2\theta, E_i, E_f)\Big|_K$ is the macroscopic double differential scattering cross section for region K. This expression ignores multiple scattering, detector efficiency corrections, and variations in sample density.

Simplifying the notation,

$$I^M \approx C\sum_{K=1}^{N}\left[A_K \frac{d^2\Sigma}{d\Omega dE}\bigg|_K f_K^M\right].$$

In principle N experimental measurements are needed in order to determine the N cross sections $\frac{d^2\Sigma}{d\Omega dE}\Big|_K$, assuming that the A_K are known and that the f_K^M can be calculated.

<u>Examples</u>

Consider the setup shown in fig. 1(a). The measured intensity may be written as

$$I^{sam} = A_1 C_1 f_1^{sam} + A_2 C_2 f_2^{sam} + A_4 C_4 f_4^{sam},$$

where

$$C_k = C\left.\frac{d^2\Sigma}{d\Omega dE}\right|_k .$$

With the sample removed the intensity is

$$I^{emp} = A_2 C_2 f_2^{emp} + A_4 C_4 f_4^{emp},$$

and with the sample container also removed we have

$$I^{cry} = A_4 C_4 f_4^{cry}.$$

Solving these three equations for C_1, we obtain

$$C_1 = \frac{1}{A_1 f_1^{sam}}\left\{ I^{sam} - I^{emp}\left(\frac{f_2^{sam}}{f_2^{emp}}\right) + I^{can}\left(\frac{f_4^{emp} f_2^{sam}}{f_4^{cry} f_2^{emp}} - \frac{f_4^{sam}}{f_4^{cry}}\right)\right\}.$$

For the simpler case of a sample in a container we would have

$$I^{sam} = A_1 C_1 f_1^{sam} + A_2 C_2 f_2^{sam}$$

and

$$I^{emp} = A_2 C_2 f_2^{emp}.$$

Hence

$$C_1 = \frac{1}{A_1 f_1^{sam}}\left\{ I^{sam} - I^{emp}\left(\frac{f_2^{sam}}{f_2^{emp}}\right)\right\}.$$

As a second example, consider the setup shown in fig. 1(b). With the sample in place the measured intensity is

$$I^{sam} = A_2 C_2 f_2^{sam} + A_3 C_3 f_3^{sam} + A_4 C_4 f_4^{sam}$$

whereas the intensity for the empty can measurement is

$$I^{emp} = A_2 C_2 f_2^{emp} + A_4 C_4 f_4^{emp}.$$

Since $C_2 = C_4$ we have enough measurements and we can solve for C_3. We obtain

$$C_3 = \frac{1}{A_3 f_3^{sam}}\left\{ I^{sam} - I^{emp}\left(\frac{A_2 f_2^{sam} + A_4 f_4^{sam}}{A_2 f_2^{emp} + A_4 f_4^{emp}}\right)\right\}.$$

Usage under *DAVE*

To use the program go to "Tools|General Tools|Self-shielding correction application."

(1) Under "Scattering Type", select a region (we shall call it k) using the slider bar. Enter its macroscopic removal cross section "sigma", i.e. Σ_k^{in}, and its radius. Check "Inelastic" if you want to do a calculation with $\Sigma_k^{out} \neq \Sigma_k^{in}$; in this case you must also enter the outgoing macroscopic removal cross section "sigma out", i.e. Σ_k^{out}. The default mode is "Elastic" in which case the "sigma

out" box content is ignored and Σ_k^{out} is set equal to Σ_k^{in}. Enter values for all regions. Ensure that unused regions have "radius" and/or "sigma" set to zero; for now the maximum number of regions is 5.

(2) Enter the lowest and highest scattering angles and the step in scattering angle. Angles are in degrees; default values are 0.0, 180.0 and 10.0.

(3) Enter the beam *half*-width W and displacement Δ; defaults are W=5.0 cm and Δ=0.0 cm respectively. Note that if the sample is fully illuminated W is at least as great as R_N, with Δ=0.0.

(4) Under "Oscillating Radial Collimator" check the "ORC" box if you want to include an
oscillating radial collimator in the calculation, in which case the four listed quantities must be entered; the default values apply to the DCS oscillating radial collimator. The default mode is "No ORC".

(5) Under "Calculation Type" enter the number of integration steps (default number is 30) or the number of Monte Carlo steps (default number is 700), depending on the type of calculation. 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.

(6) Press the appropriate button to start the calculation. The self-shielding factor $f_K^M(2\theta)$ for the specified region is plotted. Factors for other regions may be displayed using the slider bar. The transmission of the sample, averaged over the width of the beam, $T_{average}$, and the transmission of the sample through a diameter, $T_{diameter}$, are also displayed. These quantities are given by

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

and

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

respectively, where $p_k(y)$ is the path length through region k for neutrons with transverse coordinate y.

The menu bar allows you to save the results of a calculation, to show the sample geometry, to specify that you want to perform the calculation for all HFBS or DCS (!) detector angles, to print a plot of the current factors to a postscript file, and to quit.

Precision and accuracy of results

The *precision* of both types of calculation, analytic (A) and Monte Carlo (MC), improves with the number of steps. The *accuracy* of an analytic calculation also improves but in general that of an MC calculation does not change. Consider A and MC calculations that use the same input. If the calculations have very many steps they should give the same result but that result may have a systematic error because the problem has been inadequately modeled. In general there is an additional systematic error in an A calculation and this error decreases as the number of steps is increased. There is no such additional systematic error in a MC calculation. An estimate of the precision of a MC calculation performed in *asc* is given by the error bars. Note that the results for all scattering angles are correlated so the smoothness of the plotted points is not a measure of the goodness of the calculation. On the other hand a comparison of independent calculations (which necessarily use different random number seeds) is a useful measure of the MC precision. Another measure of the MC precision is obtained by comparing the exact areas A_K with MC estimates, which may be written as

$$A_k^{MC} = \frac{2W}{n}\sum_{i=1}^{n} p_k\left(\Delta + \left[2\xi_i - 1\right]W\right)$$

where n is the number of MC steps and ξ_i are random numbers uniformly distributed between 0 and 1.

In MC mode a line is printed by *asc* for each region K. The line contains R_K, A_K, A_K^{MC} and its estimated error.

Questions?

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

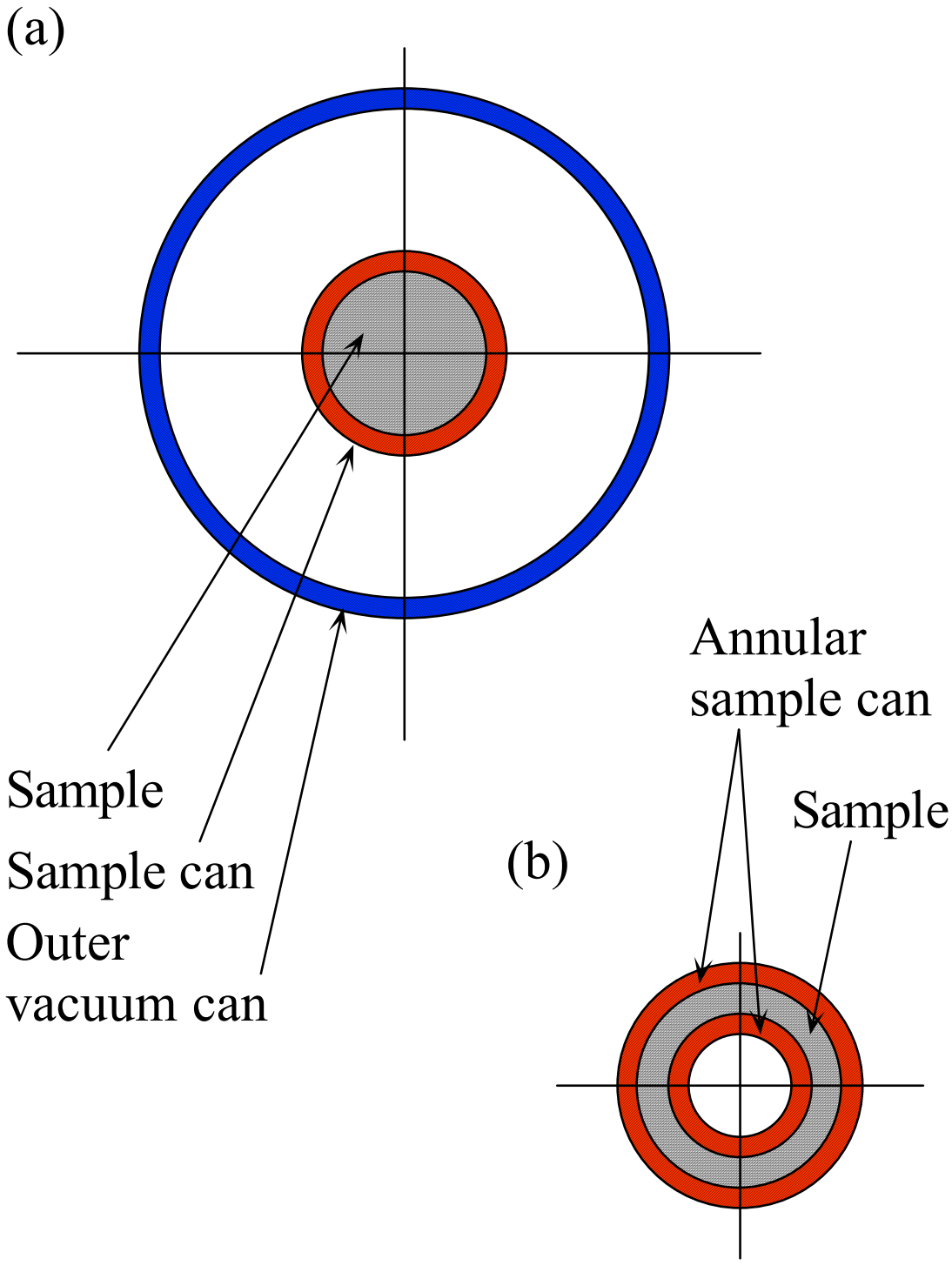
(a)
Sample
Sample can
Outer
vacuum can
(b)
Annular
sample can
Sample

Fig. 1

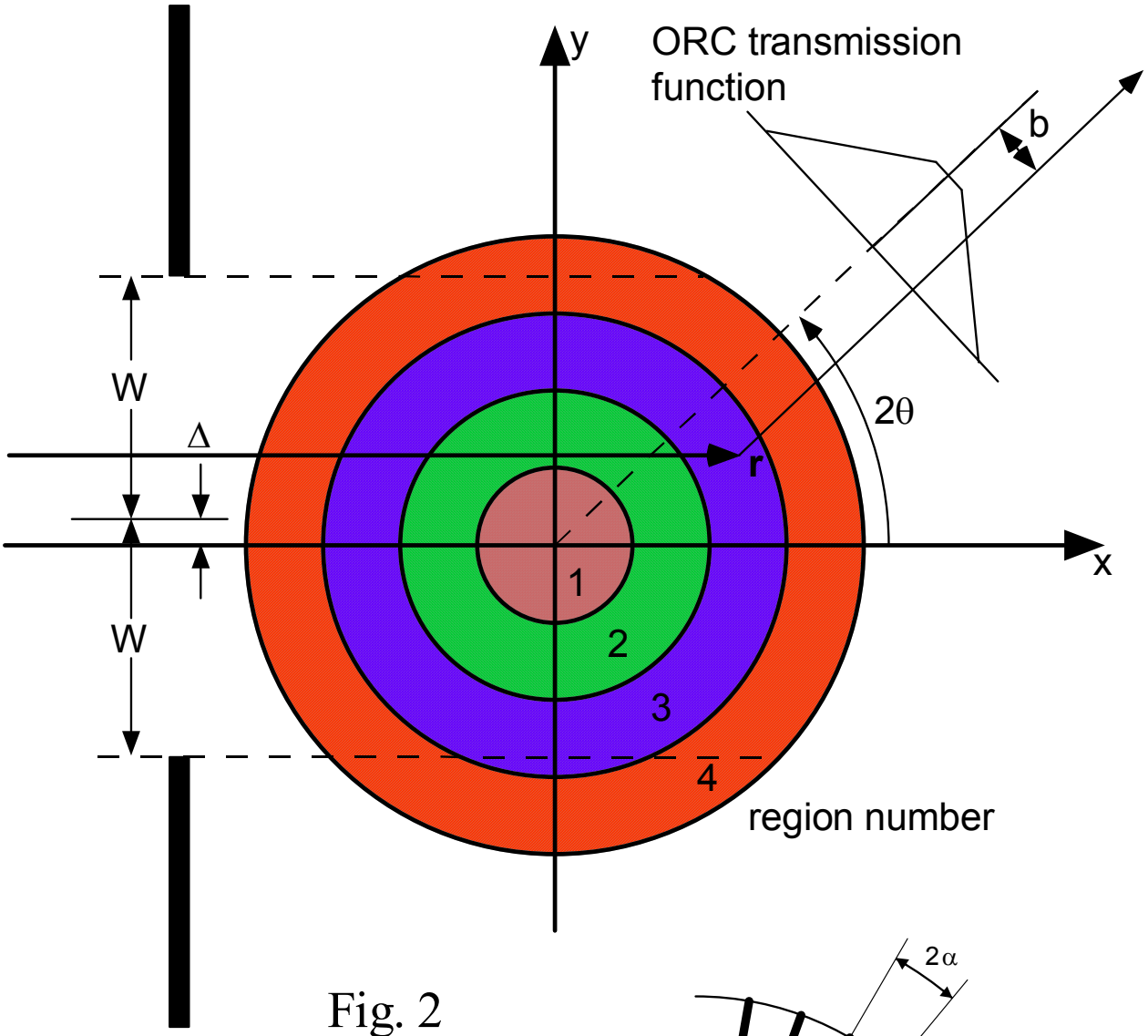
y
ORC transmission
function
b
2θ
r
x
W
Δ
W
1
2
3
4
region number

Fig. 2

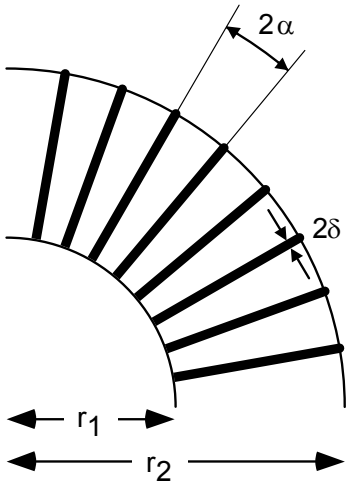
2α
2δ
r1
r2

Fig. 3