FANCY BACKGROUND SUBTRACTION, A DERIVATION WITHOUT SELF-ABSORPTION

BRIAN R. PAUW

1. Why

For strongly absorbing scattering, it is important to accurately extract the sample scattering contribution, from the contributions of the upstream and downstream sample container wall. Furthermore, the attenuation of the unscattered and scattered radiation needs to be considered. Here, a derivation is shown without considering sample self-absorption to show the general route of derivation.

2. Base definitions

2.1. **System definitions.** The scattering system is considered to consist of a three-component, sandwich-like structure (Figure 1): An upstream sample container wall, followed by the sample, followed by the downstream sample container wall. All components are considered to be plate-like in shape, with the plate normal parallel to the direct beam. Furthermore, the distance between the sample and the detector is considered to be much larger than the thickness of the sample.

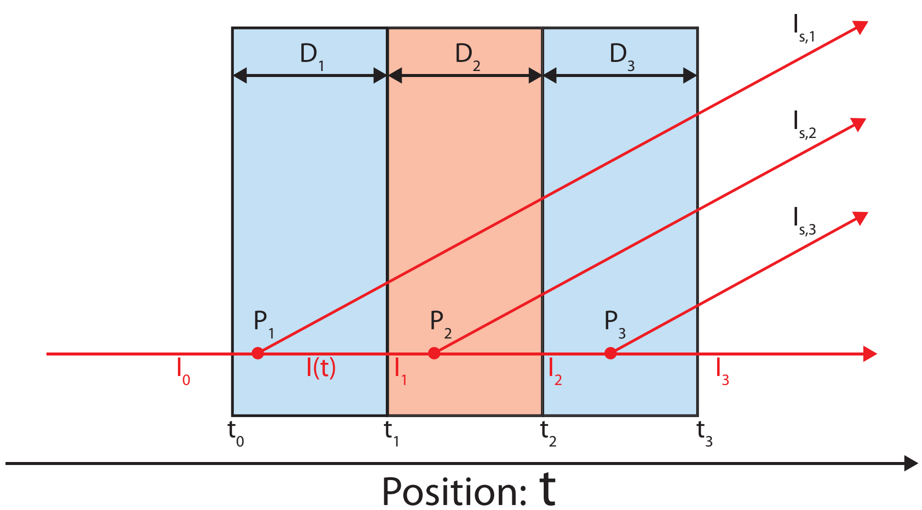

Figure 1. Schematic drawing of the scattering and absorbing elements in the X-ray beam.

2.2. **Derivation-specific assumptions.** For the initial derivation, we neglect the direction-dependent absorption of the scattered signal(s), but a future derivation may include this term (only for flat walls and phases, as the derivation thereof of round capillary-type cross-sections is ridiculously complex). It is therefore mentioned but not implemented in the final equation.

We consider three separate processes as an incident photon beam travels through a given phase: the attenuation of the incident beam by the material before a scattering event, a probability for scattering of this attenuated beam, and the attenuation of the scattered radiation by the remaining material of the phase. Each incident and scattered beam is further attenuated by the preceding and subsequent phases. We also assume that the scattering event does not significantly reduce the intensity of the remaining unscattered beam.

2.3. **Geometric definitions.** The upstream sample wall is denoted by the subscript $_1$, the sample by $_2$, and the downstream container wall by $_3$. The following definitions are made:

- D: The thickness of a phase
- t: The running variable of distance travelled through a phase
- t_0: position at the start of the upstream sample container component
- t_1: position at the start of the sample component (end of the upstream sample container component)
- t_2: position at the start of the downstream sample container component (end of sample component)
- t_3: position at the end of the downstream sample container component
- $P_n(2\theta)$: The scattering probability of phase n
- $I_0(t)$: The primary beam intensity at position t
- $I_s(t)$: The scattered intensity at position t
- I_0: The primary beam intensity
- I_1: The primary beam intensity entering the sample phase
- I_2: The primary beam intensity entering the downstream sample container component
- I_3: The primary beam intensity after absorption through all of the components
- α: The linear absorption coefficient
- 2θ: The angle of the scattered radiation
- ζ: The transmission factor of a given phase or set of phases

3. The derivation

3.1. **Absorption of the unscattered beam.** X-ray absorption is defined as:

$$I_0(t) = I_0 \exp(-2\alpha t) \quad (1)$$

The beam intensities entering and exiting the various phases therefore work out as:

$$\begin{aligned} I_1 = & \; I_0 \exp(-\alpha_1 D_1) \\ I_2 = & \; I_0 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2)\right] \\ I_3 = & \; I_0 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2 + \alpha_3 D_3\right] \end{aligned} \tag{2}$$

3.2. **Absorption of scattered beam by subsequent components.** Components in place after a scattered photon will absorb the scattered radiation with an absorption length slightly larger than the unscattered beam. The length of travel of the photon though subsequent materials is defined as:

$$l = \frac{D - t}{\cos(2\theta)} \tag{3}$$

The transmission factor ζ of scattered radiation through subsequent phases therefore is:

$$\zeta_n = \frac{I_{s,n}}{I_{s,n-1}} = \exp(-\alpha_n l) \tag{4}$$

3.3. **Intensity of the scattered beam in the scattering component.** The derivation of the scattered intensity, and direction-dependent transmission factor has been derived in the other work, where it was found to be:

$$I_1(t) = P_n I_0 \exp\left\{-\frac{\alpha}{\cos(2\theta)}\left[t\cos(2\theta) + (D - t)\right]\right\} \tag{5}$$

For the initial derivation, however, we do not consider the scattering angle-dependent increase in material pathlength, so that the term $\cos(2\theta) = 1$.

3.4. **Intensity scattered from component phases.** The scattered intensities of the individual components are defined as follows:

$$I_{sn} = I_{n-1} \int_{t_n}^{t^{n+1}} \exp(-\alpha_n t) P_n \exp\left(-\alpha_n \frac{D_n - t}{\cos(2\theta)}\right) \mathrm{d}t \tag{6}$$

With $\cos(2\theta) = 1$, this simplifies to:

$$\begin{aligned} I_{sn} = & \; I_{n-1} P_n \exp\left(-\alpha_n D_n\right) \textstyle\int_{t_n}^{t^{n+1}} 1 \mathrm{d}t \\ = & \; I_{n-1} P_n D_n \exp\left(-\alpha_n D_n\right) \end{aligned} \tag{7}$$

3.5. **Intensity scattered from the total.** The total scattered intensity is the sum of the scattering from all three components in the beam, attenuated by their subsequent phases.

$$I_s = I_{s1}\zeta_2\zeta_3 + I_{s2}\zeta_3 + I_{s3} \tag{8}$$

Substituting the components of equation 8 by with equations from 7, 2 and 4, we get for the total scattered intensity of both sandwich-cell walls and the intermediate sample:

$$
\begin{aligned}
I_s = \quad & I_0 P_1 D_1 \exp(-\alpha_1 D_1) \exp(-\alpha_2 D_2) \exp(-\alpha_3 D_3) \\
& + I_1 P_2 D_2 \exp(-\alpha_2 D_2) \exp(-\alpha_3 D_3) \\
& + I_2 P_3 D_3 \exp(-\alpha_3 D_3) \\
= \quad & I_0 P_1 D_1 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2 + \alpha_3 D_3)\right] \\
& + I_0 \exp(-\alpha_1 D_1) P_2 D_2 \exp\left[-(\alpha_2 D_2 + \alpha_3 D_3)\right] \\
& + I_0 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2)\right] P_3 D_3 \exp(-\alpha_3 D_3) \\
= \quad & I_0 P_1 D_1 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2 + \alpha_3 D_3)\right] \\
& + I_0 P_2 D_2 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2 + \alpha_3 D_3)\right] \\
& + I_0 P_3 D_3 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2 + \alpha_3 D_3)\right] \\
= \quad & I_0 \exp\left[-(\alpha_1 D_1 + \alpha_2 D_2 + \alpha_3 D_3)\right] (P_1 D_1 + P_2 D_2 + P_3 D_3)
\end{aligned} \tag{9}
$$

Assuming phases 1 and 3 are identical, this simplifies to:

$$I_s = \quad I_0 \exp\left[-(2\alpha_1 D_1 + \alpha_2 D_2)\right] (2P_1 D_1 + P_2 D_2) \tag{10}$$

3.6. **Determining** P_1**.** Before we can continue, we must find out how to determine P_1. We do this in a background measurement, by measuring the scattering from the empty cell I_b . This implies that P_2 and α_2 are both zero as this phase is not present in the measurement. We then obtain P_1 from Equation 9:

$$I_b = 2P_1 D_1 I_0 \exp(-2\alpha_1 D_1) \tag{11}$$

(NB: The first factor 2 originates from considering the upstream and downstream walls separately) So that:

$$P_1 = \frac{I_b}{2 D_1 I_0 \exp(-2\alpha_1 D_1)} \tag{12}$$

3.7. **Extracting** P_2**.** Finally, we want to find the scattering probability of phase 2 P_2 (which is what we are really after), by rearranging equation 10:

$$
\begin{aligned}
2P_1 D_1 + P_2 D_2 = \quad & \frac{I_s}{I_0 \exp[-(2\alpha_1 D_1 + \alpha_2 D_2)]} \\
P_2 = \quad & \frac{1}{D_2} \left\{ \frac{I_s}{I_0 \exp[-(2\alpha_1 D_1 + \alpha_2 D_2)]} - 2P_1 D_1 \right\} \\
= \quad & \frac{1}{D_2} \left\{ \frac{I_s}{I_0 \exp[-(2\alpha_1 D_1 + \alpha_2 D_2)]} - \frac{I_b}{I_0 \exp(-2\alpha_1 D_1)} \right\}
\end{aligned} \tag{13}
$$

Substituting the transmission factors for the empty cell $\zeta_1 = \exp(-2\alpha_1 D_1)$ and cell plus sample $\zeta_{1+2} = \exp\left[-(2\alpha_1 D_1 + \alpha_2 D_2)\right]$, we can see that we arrive at the (more or less) standard background subtraction calculation:

$$P_2 = \frac{1}{D_2} \left\{ \frac{I_s}{I_0 \zeta_{1+2}} - \frac{I_b}{I_0 \zeta_1} \right\} \tag{14}$$

So, after this work, we find out that even when we thoroughly consider the scattering process of a sample sandwiched between two sample cell walls, we arrive at a simple equation for determining the sample scattering probability from the total measured intensity.

4. Final remarks

There are interesting aspects when we use this background subtraction equation in practice. Firstly, we find that it is not necessary to determine the sample cell wall thickness D_1. Secondly, both the sample measurement and the background measurement are normalised to the thickness of the sample phase D_2 only. Lastly, it should be noted that this is, of course, only valid if the same sample cell is used for both the background and the sample measurement.