Procedure for the determination of effective
temperatures employing VESUVIO spectrometer

J Dawidowski¹, L A Rodríguez Palomino¹, G Romanelli², and M
Krzystyniak²
¹Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Comisión Nacional
de Energía Atómica-Universidad Nacional de Cuyo, Argentina
²ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom
E-mail: jdawidowski@gmail.com

Abstract. We describe the procedure to determine effective temperatures employing the data collected by the detectors of the VESUVIO spectrometer (ISIS pulsed neutron source), employing the Deep Inelastic Neutron Scattering technique. A scheme to group the detectors is proposed, based on their positions and angular ranges, in order to add their spectra and improve the statistics. We show the details of all the corrections that must be made on the raw experimental data to reach the spectra on which the desired effective temperatures can be fitted. Most of the correction stages require ad-hoc auxiliary simulations by the Monte Carlo method, that were devised and described in previous papers. The corrections, that involve background subtraction, empty cell subtraction, and multiple scattering corrections, are described in detail. The efficiencies of the defined detector groups are determined, and employed in the expressions used in data fitting. Data treatment steps performed in hydrogenated and deuterated alcohols, are shown as examples of application of this procedure.

1. Introduction
The knowledge of the kinetic energy of the atoms in condensed matter is a subject of primary interest in Neutron Physics. This is because this observable determines properties of interest, such as the width of nuclear neutron resonances (through the Doppler broadening) [1], or the spectrum shape produced by neutron moderators [2], among others often related to Nuclear Engineering calculations. In all the mentioned cases, a basic parameter that is necessary to know is the mean value of the kinetic energy, which is determined by the thermodynamic temperature as well as the dynamic properties of the system. The mean kinetic energy is often referred to as the effective temperature, depending upon the scope of a given application. While dependent on the thermodynamic temperature, the effective temperature of the atoms that compose a system is also a function of the vibrational densities of states [3, 4].

In Nuclear Engineering it is usual to determine the effective temperatures indirectly from models of frequency spectra [5]. With Deep Inelastic Neutron Scattering (DINS) it is possible to measure directly the effective temperatures of each atomic species composing a system, since it is a mass-resolved technique [6]. This provides a unique tool to access experimentally this observable.
The VESUVIO spectrometer (ISIS, Rutherford Appleton Laboratory, UK) has the possibility to cover a wide range of scattering angles, with 64 detectors in forward scattering and 132 detectors in backscattering directions. Originally devised to study the detail of the momentum distributions profiles [7], it also proved to be a useful tool to determine neutron total cross sections as a function of energy by employing its transmission monitor [9]. In this paper, we address the situation when no specific details of the Compton profile are sought, and only the mean value of the kinetic energy needs to be obtained. In such cases, reliable results can be obtained by adding the signal of groups of detectors, with the advantage of improving the statistics, a common practice among the various neutron scattering spectrometers. A different approach to the problem is to transform the detector signals to the variable $y$ (West scaling [6]), and add the spectra afterwards. However as shown in Ref. [10] the $y$-scaling (associated with the Convolution Approximation) is an approximation, that consists in considering that the filter has a single well-defined energy in the passage from time of flight to $y$, while the uncertainties associated with the energy width of the filter and others are packed in the resolution function. We showed that there are discrepancies of this approximation from the exact expression noticeable for the case of light nuclei. In this paper we decided to avoid such intermediate uncertainty, by using the exact expression, adding the signals of the individual detectors in the time-of-flight variable at the expense of reducing the angular resolution.

As the purpose of this paper is mainly methodological, we will focus our attention on the procedure to treat the data of the detector groups, from the raw data to the final effective temperature fitted from the profiles, along the lines traced in Ref. [5]. The systems studied are a set of normal and deuterated alcohols, whose total cross sections were previously determined [9]. The systematic study of the effective temperatures of these systems will be left for a forthcoming paper.

2. Experimental

The experiments described in this work were carried out at the VESUVIO spectrometer, placed at target station 1 (TS1) of the ISIS pulsed neutron and muon source at the Rutherford Appleton Laboratory (United Kingdom). A general sketch of VESUVIO is shown in Fig. 1. The forward scattering detectors are yttrium aluminum perovskite (YAP) $\gamma$-ray detectors (S135 to S198), and the backscattering detectors (S3 to S134) are $^6$Li-doped glass scintillators. The analyzer filters are movable $^{197}$Au foils that allow filter-in and filter-out measurements, employed to perform the single-difference (SD) technique. A thorough description of the system and its operation can be found in Ref. [7].

In this paper we will refer to measurements performed on hydrogenated and deuterated alcohols in two batches. The samples were liquid high-purity 1-propanol (CH$_3$CH$_2$CH$_2$OH), 2-propanol (CH$_3$CHOHCH$_3$), n-butanol (CH$_3$CH$_2$CH$_2$CH$_3$OH), 1-propanol-OD (CH$_3$CH$_2$CH$_2$OD), 2-propanol-D8 (CD$_3$CDODCD$_3$) and n-butanol-D10 (CD$_3$CD$_2$CD$_2$CD$_2$OD), bought from Sigma Aldrich [8], with 99% deuteration in the case of the last three [9]. The samples were in the liquid state kept at room temperature, held into aluminum flat cells of square sections 65 mm inner side and 90 mm outer side. The thicknesses were 1.5 mm in the case of normal and 2 mm in the case of the deuterated samples.

The spectra were recorded as a function of the time of flight, and treated with programs based on the Open Genie display and data analysis suite, developed for the neutron scattering instruments at the ISIS facility [11].

3. Data treatment

3.1. Fundamentals

One of the purposes of this work is to integrate the spectra of several detectors to improve the statistics. The difference spectra is the usual working magnitude in DINS experiments and
Figure 1. VESUVIO general setup, showing the forward scattering and backscattering detectors.

consists in the ‘filter-out’ minus ‘filter-in’ spectra. We will consider the sum of the spectra of detectors at scattering angles $\theta_i$, in an angular range such that $\theta_{\text{inf}} < \theta_i < \theta_{\text{sup}}$. Then, the expression of the recorded spectra is [12]

$$
c(t) = \sum_{\theta_i = \theta_{\text{inf}}}^{\theta_{\text{sup}}} \int_{E_{\text{inf}}}^{\infty} dE_0 \Phi(E_0) \frac{d^2\sigma(E_0, E, \theta_i)}{d\Omega dE} \varepsilon(E) \left[ 1 - e^{-nT\sigma_F(E)} \right] \left\| \frac{\partial E}{\partial t} \right\| \Delta\Omega.
$$

In Eq. (1), $\Phi(E_0)$ is the energy dependent incident neutron flux, $\frac{d^2\sigma(E_0, E, \theta_i)}{d\Omega dE}$ is the double-differential cross section of the sample, and $\varepsilon(E)$ is the detector group efficiency. The expression $\left[ 1 - e^{-nT\sigma_F(E)} \right]$ corresponds to the absorption probability of the resonant filter, characterized by a number density $n$, a thickness $T$, and a total cross section $\sigma_F(E)$. In the present work, gold foils were employed with a thickness of 0.0125 mm for the forward scattering and 0.05 mm for the backward scattering detectors. Finally, $\Delta\Omega$ is the solid angle subtended by a detector. The lower limit of integration $E_{\text{inf}}$ is determined by kinematic conditions, while the sum spans over the signals of all the detectors in the considered angular range. It is worth noting that Eq. (1) is strictly valid for single scattering. For a real sample of finite dimensions, the total count rate recorded by the detectors is composed by singly and multiply scattered neutrons. The main route of calculation is by Monte Carlo simulations [12], as it will be shown in Sect. 4.
Table 1. Definition of the 10 detector groups in the forward scattering direction. The number of detectors in each group and the lower and upper angular limits ($\theta_{\text{inf}}$ and $\theta_{\text{sup}}$ of Eq. (1) in degrees) are indicated.

| Group | Number of detectors | $\theta_{\text{inf}}$ ($^\circ$) | $\theta_{\text{sup}}$ ($^\circ$) |
|-------|---------------------|-------------------------------|-------------------------------|
| 1     | 4                   | 31.7                          | 35.0                          |
| 2     | 6                   | 36.9                          | 39.4                          |
| 3     | 6                   | 41.0                          | 45.7                          |
| 4     | 6                   | 41.9                          | 45.9                          |
| 5     | 4                   | 47.0                          | 47.7                          |
| 6     | 8                   | 50.7                          | 54.1                          |
| 7     | 6                   | 50.7                          | 54.7                          |
| 8     | 8                   | 55.4                          | 60.1                          |
| 9     | 6                   | 60.6                          | 63.9                          |
| 10    | 10                  | 65.0                          | 69.7                          |

Table 2. Definition of the 3 detector groups in backscattering direction. The number of detectors in each group and the lower and upper angular limits ($\theta_{\text{inf}}$ and $\theta_{\text{sup}}$ of Eq. (1) in degrees) are indicated.

| Group | Number of detectors | $\theta_{\text{inf}}$ ($^\circ$) | $\theta_{\text{sup}}$ ($^\circ$) |
|-------|---------------------|-------------------------------|-------------------------------|
| 1     | 21                  | 152.5                         | 165.9                         |
| 2     | 51                  | 139.5                         | 151.2                         |
| 3     | 60                  | 131.0                         | 139.6                         |

Eq. (1) will serve as the basic expression to fit the effective temperatures to the spectra, after the experimental corrections below described are applied.

3.2. Detectors grouping

As mentioned above we defined detector groups in order to add their signals together. The criteria followed to include detectors in a group were to chose

- detectors placed at neighboring scattering angles,
- detectors placed at similar distances to the sample.

For the forward scattering detectors in Fig 1 we observe that there are basically two typical sample-detector distances. Fig. 2 shows the detectors layout as seen from the sample position along the beam direction. The angular range covered by the detectors is roughly from 31° to 70°. Applying the above mentioned criteria, 10 detector groups are defined and shown in different colors. Table 1 shows the angular limits of each group.

The backscattering detectors are arranged on a plane (as shown in Fig. 1). Fig. 3 shows the detectors layout as seen from the sample position in the beam direction. The angular range covered by the detectors is roughly from 131° to 166°. In this case 3 detector groups are defined, which are shown in different colors. Table 2 shows the angular limits of each group.

Fig. 4 illustrates the resulting difference spectra (‘filter-out’ minus ‘filter-in’) for the defined groups in forward and backward scattering, taking as examples the cases of 2-propanol(H) and 2-propanol(D) respectively.
3.3. Determination of the detector groups’ efficiencies

In Eq. (1), the efficiency of the detector group is a required quantity to be known when calculating the time-of-flight spectra $c(t)$. In practice, this determination is made by comparing a spectrum measured with the detector whose efficiency we want to know, with the same spectrum measured with a detector of known efficiency. In this case, we firstly measured the incident spectrum $\Phi(E)$, with the transmitted beam monitor S2, shown in Fig. 1, a $^6$Li-doped glass scintillator of known efficiency. In the case of a detector group, $\Phi(E)$ was determined by measuring the spectrum of a lead target (placed in the sample position), that was considered an elastic and isotropic scatterer as commented in Ref. [12]. If $D_{\text{Pb}}(E)$ is the measured Pb spectrum (after subtracting the background, measured by leaving empty the sample position), the efficiency $\varepsilon(E)$ can be determined from the relation

$$D_{\text{Pb}}(E) = \varepsilon(E)\Phi(E).$$

Since this method to determine the efficiency is based on the measurement of two spectra, and none of them are absolutely measured, we obtain the shape of the efficiency curve and not its absolute value (as in the case of the spectrum), therefore leaving an undetermined multiplicative constant in Eq. (1).

In Fig. 5 we illustrate the determination of the efficiency for the specific case of detector
Figure 3. VESUVIO backward scattering detectors as seen from the sample position in the direction opposed to the beam, showing their numbering and the proposed 3 groups employed for the analysis in this work. The colors indicate the group numbers.

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Perelli-Cippo et al. [15] by means of polynomial functions. After treating different kinds of samples, two main conclusions can be drawn on the background on the difference spectra:

(i) It is filter-dependent. It means that the ‘filter-out’ minus ‘filter-in’ spectrum, leaves a remaining background that is not canceled by the difference.

(ii) It is sample dependent. The intensity and shape of the background depends on the scattering power of the sample. Thus, we distinguished two different behaviors depending on whether the samples are hydrogenated or deuterated.

In practice, we proceeded as follows. The hydrogenated and the deuterated samples data sets were treated separately, searching a common background spectrum for each one. The measured difference spectra were compared with the total Monte Carlo calculated profiles that will be described in Sect. 4. The difference between the measured and simulated spectra was ascribed to the background.

The process is depicted in Fig. 6, where we focus on the hydrogenated alcohols spectra of group 2 of backscattering detectors (see Fig 3). In its right frame we show the experimental difference spectra (in full lines), together with the total Monte Carlo simulations. The apparent differences between measured and simulated spectra are due to the backgrounds, that are shown in the right frame, for each sample. Their great similitude allows us to represent them by a single fourth degree polynomial (drawn in blue line).

Fig. 7 depicts the process of background corrections for the hydrogenated alcohols in detector group 2 (backscattering). The upper row shows the measured spectra, together with the polynomial background and the corrected spectra after background subtraction. The lower
Figure 5. Left: Incident neutron spectrum (measured with transmission detector S2 and corrected by its efficiency), and Pb sample and background spectra (measured with forward scattering detector group 10). Right: the function $\varepsilon(E)$ (black) calculated from the spectra in the right frame, and the adopted efficiency function (red continuous and dotted lines, see text for details).

row shows the corrected data compared with the Monte Carlo simulations. The good agreement shown serves as a consistency check of the procedure.

3.5. Empty cell subtractions
When working with samples that require the use of a container such as for liquids, gases or powders, empty cell measurements are normally made, in order to subtract their signal. This can not be done directly due to the attenuation of the beam in the sample and in the cell, and the multiple scattering, which makes the contribution of the full cell different from that of the empty cell. Paalman and Pings formulated analytical expressions [16] for empty-cell subtraction in the case of X-ray scattering, and well-defined sample geometries. As commented in Ref. [17], the method is not well suited for the case of neutron scattering (although its use is common practice), because only elastic scattering is considered, (and therefore the cross sections are constants). This is usually far from the real case with neutrons, for which multiple inelastic scattering may be important.

The empty-cell subtraction we consider here, relies on Monte Carlo simulations (described in Sect. 4), of the sample-cell (SC), empty cell (C) and sample-only (S) systems. Thus, we calculate the spectra $C_{SC}(t)$, $C_{S}(t)$, $C_{C}(t)$, and define the cell subtraction factor

$$f_C(t) = \frac{C_{SC}(t) - C_{S}(t)}{C_{C}(t)},$$

that establishes the relation

$$C_{S}(t) = C_{SC}(t) - f_C(t)C_{C}(t).$$
Figure 6. Left: In full lines the experimental difference spectra of the Hydrogenated alcohols for detector group 2 in backscattering. In dashed lines the corresponding total Monte Carlo simulations (with the same color convention as for the experimental). Right: The differences between the experimental and the calculated spectra, showing that they can be approximately described by a common background (with the same color convention indicating the samples) The blue thick line is the fitted polynomial function employed to represent the background.

The next step is to apply the same relation to the experimental data, $\mathcal{E}_{SC}(t)$ and $\mathcal{E}_C(t)$, which provides the sought way to subtract the cell

$$\mathcal{E}_S(t) = \mathcal{E}_{SC}(t) - f_C(t)\mathcal{E}_C(t),$$

where $f_C$ is calculated from (3), and $\mathcal{E}_{SC}$ and $\mathcal{E}_C$ are measured. The precision of the method depends on the accuracy of the description of the scattering cross sections and the mean free paths as a function of the energy in the Monte Carlo code.

We found that the factors $f_C(t)$ can be represented by one function for the hydrogenated and another for the deuterated samples, regardless the detector group. In Fig. 8 we illustrate such results for the case of a forward and a backward scattering group. We also show the 7th degree polynomials employed to represent $f_C(t)$, together with values of $f_C(t)$ calculated from Eq. (3) with Monte Carlo results in some of the studied systems. Although noticeable statistical fluctuations are evident, the calculations allow a proper definition of the polynomials. In the insets of Fig. 8, we show two representative Monte Carlo results for sample-cell, empty cell and sample-only systems in hydrogenated n-butanol, for forward (left) and backward scattering (right). The proximity of the polynomial to a value about 1 for for the deuterated samples, is a consequence of the transparency of the sample, in which case Eq. (5) is a direct subtraction of the empty cell.

Fig. 9 shows an application of the proposed cell subtraction procedure, for the cases of hydrogenated and deuterated 2-propanol for detector group 3 in backscattering. Rather than the raw experimental empty cell spectra, we fitted Lorentzian functions (shown in red) to avoid amplifying the noise in the subtraction. The blue line indicates the term $f_C(t)\mathcal{E}_C(t)$ of Eq. (5), and the orange line shows the cell-subtracted spectra.
Figure 7. Background corrections for the hydrogenated alcohols detector group 2 in backscattering. In the upper row of frames we show the measured spectra (black lines), the background fitted with a single fourth-degree polynomial (red lines), and the resulting spectra after background subtraction (green lines). In the lower row of frames we show the spectra after background subtraction (black lines) compared with the total Monte Carlo simulations (red lines).

4. Monte Carlo simulations
Monte Carlo simulations have the dual purpose of correcting the experimental data for multiple scattering, attenuation, and detector efficiency effects, and also helping in the analysis of the background as shown in Sects. 3.4 and 5. A detailed account of the Monte Carlo procedure employed can be found in Ref. [18], where the reader is referred for further details. As above referred, the Monte Carlo procedure requires the knowledge of the incident spectrum and the detector efficiency, together with instrumental parameters such as the sample and filter geometries and their total cross sections as a function of the energy. An essential input for the Monte Carlo simulations are the total cross sections of the alcohols and their synthetic frequency spectra that govern the dynamics of the modeled systems. Both subjects were extensively studied for the alcohols presented in this work in Ref. [9]. Finally, the filter analyzer absorption cross section as a function of energy is read from absorption cross section tables, that can be obtained from Ref. [19].

In Fig. 10 we show the comparison of the experimental and Monte Carlo data of normal and deuterated 2-propanol for the group number 10 in forward position (left) and number 3 in backward position (right), respectively. The good agreement observed guarantees the suitability of the Monte Carlo simulations for the aforementioned uses.

5. Multiple scattering corrections
As extensively treated in Ref. [9], we correct the experimental data by beam attenuation and multiple scattering effects, by Monte Carlo simulations (described in Sect. 4). In the present case we made such corrections after subtracting the cell effects as described in Sect...
Figure 8. The cell subtraction factor $f_C(t)$ calculated from Monte Carlo results for hydrogenated and deuterated alcohols and different detector groups, in forward scattering (left) and backward scattering (right). The results are fitted with 7th degree polynomials for each type of sample. Insets: Monte Carlo results for n-butanol (H) used to determine the factors.

3.5. Therefore, the Monte Carlo simulations for this corrections were made only on the sample system (without considering the cell). The attenuation correction factor $H(t)$ is defined as ratio of the detected singly-scattered neutrons to the total singly-scattered neutrons spectra, and the multiple scattering correction factor $M(t)$ is defined as the ratio the detected singly-scattered neutrons to the total scattered neutrons spectra [9]. The experimental data $E(t)$ are then corrected by

$$E_{\text{corr}}(t) = \frac{M(t)E(t)}{H(t)} = F(t)E(t),$$

where we defined a single factor $F(t) = \frac{M(t)}{H(t)}$ that we call experimental correction factor.

As examples, in Fig. 11 we show the experimental data for the hydrogenated samples for group 10 in forward scattering (frame (a)) and the deuterated samples for group 3 in backscattering (frame (b)), and their corresponding correction factors determined by simulations (insets). It is worth to notice that these factors are very similar for each family of samples, so only one of them was shown. The right frames show the data corrected by these effects.

Upon reaching this instance we summarize the corrections made on the raw data:

- Background subtraction
- Empty cell effects
- Beam attenuation
- Multiple scattering.
Figure 9. Empty cell spectra subtraction for hydrogenated and deuterated 2-propanol for detector group 3 in backscattering. The empty cell spectra are measured and fitted with a Lorentzian function (red line). The blue line indicates the term $f_C(t)\mathcal{E}_C(t)$ of Eq. (5).

Figure 10. Comparison of experimental and Monte Carlo data of hydrogenated 2-propanol for the detector group number 10 in forward scattering (left) and deuterated 2-propanol for the detector group number 3 in backward scattering (right). The detail of the single scattering and multiple scattering components is shown.
Figure 11. The frames (a) and (b) show the experimental data after background and can subtraction for detector-group 10 (forward scattering, hydrogenated samples) and group 3 (backscattering, deuterated samples), respectively. Their corresponding correction factors defined in Eq. (6) and determined by Monte Carlo simulations are shown in the insets. The frames (c) and (d) show the data corrected by multiple scattering, attenuation and efficiency. Therefore, the data on the right frames of Fig. 11 are already corrected by the aforementioned effects, and are ready to be used in the analysis of effective temperatures.

6. Data fitting
Fig. 12 shows representative measured profiles of deuterated 2-propanol (group 1 and 3 of backscattering detectors) together with the corresponding fitted curves and the separate contributions of D, C and O, employing Eq. (1). The double-differential cross section of the
system was modeled by a mixture of gases with effective temperatures, as described in Ref. [5].

![Graphs showing deuterated 2-propanol profiles](image)

**Figure 12.** Profiles of deuterated 2-propanol, at group 1 (left) and group 3 (right) of backscattering detectors corrected by the experimental effects described in this work together with the corresponding fitted curves and the separate contributions of D, C and O.

A good precision in the determination of the deuterium effective temperature is found (60.2 ± 0.1 meV for the group-1 spectrum and 60.3 ± 0.1 meV for the group-3 spectrum), whereas the superposition of peaks prevented us from achieving acceptable values for C and O. Further results of effective temperatures of alcohols will be shown elsewhere.

7. Conclusions
In this work we have shown a procedure to treat VESUVIO data from groups of detectors, as a way to improve the statistics for the determination of effective temperatures of the atoms that
compose the sample. A scheme was proposed in which the 64 forward detectors were grouped into 10 groups, and the 132 backward detectors were grouped into 3 groups. The knowledge of effective temperatures is relevant in Nuclear Engineering and the method shown here allows a direct experimental way to obtain these parameters.

Raw experimental data must go through an instrumental characterization such as the detector groups efficiency determination, and several stages of corrections, before being ready to be analyzed. To show such stages was the purpose of this work.

All the correction steps were facilitated by Monte Carlo simulations. The determination of the residual background characteristic of the instrument was obtained through the comparison of spectra of similar samples and their corresponding Monte Carlo simulations. To suitably subtract the empty cell spectrum, Monte Carlo simulations were carried out to determine the cell attenuation factor to be used in the subtraction. Finally the Monte Carlo simulations were used in their well-known role to determine the effects of multiple scattering and attenuation, to correct the data.

To be able to perform adequate Monte Carlo simulations, a prior knowledge of the system to be modeled and the experimental parameters of the instrument are required. Key parameters to be included in the simulations are the total cross sections of the studied systems as a function of the energy, also available as output of a VESUVIO experiment through the information given by transmission detector S2, provided the incident spectrum is also measured.

The procedure shown allowed us to obtain the profiles ready to be analyzed. The fitted effective temperatures shown as examples evidence satisfactory precision in the results. A systematic study of the effective temperatures of the studied hydrogenated and deuterated alcohols will be shown in a forthcoming paper.

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