Notes on Using the "Water" Excel Spreadsheet
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This spreadsheet was designed to illustrate how quasielastic neutron scattering spectra changed as time constants (diffusion constants), molecule geometry, momentum transfer, and instrument resolution were varied. The model that is coded has been used historically for water diffusion.[1-3] This model has three components: a Debye-Waller term to account for local, harmonic oscillations ($e^{-\langle u^2 \rangle Q^2/3}$); a translational diffusion term, *T(Q,ω)*; and *finally, a rotational term, R(Q,ω), that captures reorientations of the water molecule.* Q and ω are the momentum and energy transfers, respectively. These terms are taken as independent of one another and the resulting dynamic structure factor, *S(Q,ω)*, is taken as the convolution of the individual terms:

$$S(Q,\omega) = e^{-\langle u^2 \rangle Q^2/3}\, T(Q,\omega) \otimes R(Q,\omega) \tag{1}$$

The translational term is given as a Lorentzian

$$T(Q,\omega) = \frac{1}{\pi}\frac{\Gamma(Q)}{\omega^2 + \Gamma^2(Q)} \tag{2}$$

For jump diffusion, the Lorentzian HWHM, $\Gamma(Q)$, is given by

$$\Gamma(Q) = \frac{D_t Q^2}{1 + D_t Q^2 \tau_t} \tag{3}$$

where D_t is the translational diffusion constant and τ_t is the mean residence time between jumps. These are related to the mean jump distance, l, via

$$D_t = \frac{\langle l^2 \rangle}{6\tau_t} \tag{4}$$

The rotational term is modeled as diffusion on the surface of a sphere

$$R(Q,\omega) = j_0^2(Qa)\delta(\omega) + \frac{1}{\pi}\sum_{i=1}^{\infty}(2i+1)j_i^2(Qa)\frac{i(i+1)D_r}{(i(i+1)D_r)^2 + \omega^2} \tag{5}$$

where a is the sphere radius, D_r is the rotational diffusion constant, and the j_i are spherical Bessel functions. The rotational correlation time, t_r, is related to the rotational diffusion constant as

$$\tau_r = \frac{1}{6D_r}$$	(6)

The parameters that describe the dynamics are then D_t τ_t, t_r, a, and $\langle u^2 \rangle^{0.5}$. A particular value for the momentum transfer may be given. In addition, the instrument resolution function is modeled as a Gaussian whose FWHM is also specified in the spreadsheet. The jump length, l, is calculated from D_t and τ_t according to Eq. (4) and is presented for information only, it is not entered directly into the spread sheet.

The model is coded in a macro written in Visual Basic that runs behind the spreadsheet whenever the "RUN" button is clicked. The macro can be examined by clicking on Tools-Macro-Macros and then selecting the "Run_QNS_Water_model" and then click the "Edit" button. Changes to the parameters in the yellow boxes may be made by clicking on the box, entering a new value and then hit the "Enter" key. This will change the value in the box, hitting the "Run" button will then launch the Macro and a new plot will be generated using the new parameter values. You must have the security setting for Macros set to no higher than "Medium" and "enable Macros" when you open the spreadsheet.

References

[1] J. Teixeira, M. C. Bellissent-Funel, S. –H. Chen, and A. J. Dianoux, Phys. Rev. A **31** 1913 (1985).

[2] M. R. Harpham, B. M. Ladanyi, N. E. Levinger, and K. W. Herwig, J. Chem. Phys. **121**, 7855 (2004).

[3] H. N. Bordallo, K. W. Herwig, B. M. Luther, and N. E. Levinger, J. Chem. Phys. **121**, 12457 (2004).