diwanalr: An R data analysis package for diffusing-wave spectroscopy

Peter J Watkins[1]

1 Commonwealth Scientific and Industrial Research Organisation

DOI: 10.21105/joss.00947

Software

- Review
- Repository
- Archive

Submitted: 17 July 2018
Published: 24 June 2019

Summary

The **diwanalr** (**di**ffusing-**wa**ve spectroscopy (DWS) **anal**ysis using **R**) package contains a number of functions suitable for analysing DWS data. DWS is an optical technique derived from dynamic light scattering which studies the dynamics of scattered light (Wietz & Pine, 1993). If carefully calibrated, DWS allows the quantitative measurement of microscopic motion in a soft material, which can be used with micro-rheology to determine the rheological properties of such a complex medium.

DWS has been applied to the analysis of food systems. Some examples include understanding the dynamics of emulsion systems (e.g. fat in water) such as mayonnaise (Kim, Șenbil, Zhang, Scheffold, & Mason, 2019) along with the gellation of food products (Alexander, Corredig, & Dalgleish, 2006).

DWS also has practical applications in the pharmaceutical and cosmetic industries as well (Reufer et al., 2014).

In some instances, the analysis of data resulting from DWS measurements can be tedious depending on, for example, the use of spreadsheets for numerical analysis, or multiple software packages (Niederquell, Machado, & Kuentz, 2017). The **diwanalr** package has been developed as an alternative approach, allowing data analysis to be readily performed using a single software package, within R. The package has a set of functions which can be readily and seamlessly deployed after the measurement of data. Further functionality can be added to the package as required.

The package utilises four R packages (*dplyr*, *ggplot2*, *tibble* and *tidyr*) in its implementation.

Background

At present, the package can be deployed to determine the viscoelastic, storage and loss moduli of a system using data, consisting of time and related values from the temporal autocorrelation function, $g_2(t)$. The latter is related to the intensity autocorrelation function, $g_1(t)$, by the Seigert equation, where $g_2(t) = 1 + |g_1(t)|^2$ (Seigert, 1943). The $g_1(t)$ values are used to determine the mean square displacement (MSD) for transmission geometry by solving the relationship (Wietz & Pine, 1993):

$$g_1(t) \approx \frac{(\frac{L}{l*}+\frac{4}{3})\sqrt{\frac{6t}{\tau}}}{(1+\frac{8t}{3\tau})sinh[\frac{L}{l*}\sqrt{\frac{6t}{\tau}}]+\frac{4}{3}\sqrt{\frac{6t}{\tau}}cosh[\frac{L}{l*}\sqrt{\frac{6t}{\tau}}]}$$

which are then used to calculate the *viscoelastic* modulus, and related *storage* and *loss* moduli for the system under study.

Acknowledgement

The author wishes to acknowledge, and credit, W. N. (Bill) Venables for optimising the code for the MSD determination.

References

Alexander, M., Corredig, M., & Dalgleish, D. G. (2006). Diffusing wave spectroscopy of gelling food systems: The importance of the photon transport mean free path (l*) parameter. *Food Hydrocolloids*, *20*(2), 325–331. doi:https://doi.org/10.1016/j.foodhyd.2005.02.021

Kim, H. S., Şenbil, N., Zhang, C., Scheffold, F., & Mason, T. G. (2019). Diffusing wave microrheology of highly scattering concentrated monodisperse emulsions. *Proceedings of the National Academy of Sciences*, *116*(16), 7766–7771. doi:10.1073/pnas.1817029116

Niederquell, A., Machado, A. H. E., & Kuentz, M. (2017). A diffusing wave spectroscopy study of pharmaceutical emulsions for physical stability assessment. *International Journal of Pharmaceutics*, *530*(1), 213–223. doi:https://doi.org/10.1016/j.ijpharm.2017.07.038

Reufer, M., Machado, A. H. E., Niederquell, A., Bohnenblust, K., Müller, B., Völker, A. C., & Kuentz, M. (2014). Introducing diffusing wave spectroscopy as a process analytical tool for pharmaceutical emulsion manufacturing. *Journal of Pharmaceutical Sciences*, *103*(12), 3902–3913. doi:https://doi.org/10.1002/jps.24197

Seigert, A. J. (1943). MIT Radiation Laboratory Report, No. 465.

Wietz, D. A., & Pine, D. J. (1993). Diffusing-wave Spectroscopy. In W. Brown (Ed.), *Dynamic light scattering* (pp. 652–720). Oxford University Press.