

# diffusion-fundamentals

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## Modelling Aroma Release from Silica Sol-Gel Particles Using Self-Diffusion Data Obtained Under Magic Angle Spinning Conditions

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### 1. Introduction

Silica sol-gel particles have a possible use as aroma delivery systems in the food and cosmetic industries. We have studied the kinetics of aroma release from silica sol-gel particles in ethanol by UV-VIS spectroscopy [1]. The release kinetics were modelled, taking into account the physical properties of the particles and the calculated self-diffusion coefficient of the aroma molecules. Through the use of self-diffusion NMR, coupled with magic angle spinning we have also measured the diffusion properties of the aroma molecules directly. The diffusion values obtained were successfully used to model the UV-VIS kinetic data. In this poster we discuss the potential of obtaining diffusion data under magic angle spinning conditions in both model and real porous media systems.

### 2. Magic Angle Self-Diffusion Results

Using a Bruker HR-MAS probe with a field gradient oriented along the magic angle we were able to obtain the self-diffusion coefficient of simple water and water surrounding 100  $\mu\text{m}$  polystyrene beads using a simple pulsed-gradient stimulated echo (PGSTE) experiment. In the figure we have the echo response of the PGSTE experiment showing very good linearity for simple water [(a) & (b)] and water surrounding beads [(c) & (d)] while spinning the sample at 1.5 kHz. Further experiments were performed to measure the long time diffusion limit response of the water signal surrounding the beads that should be

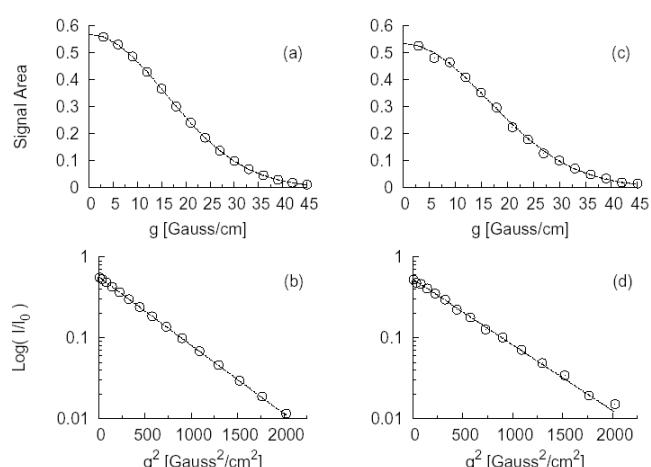


Fig. 1 Self-diffusion results obtained under magic angle spinning for water alone (a,b) & water surrounding 100  $\mu\text{m}$  polystyrene beads (c,d).

solely dependent on the bead size and packing. After further validation of the experimental set-up we have investigated a number of aromas encapsulated in silica sol-gel particles. The intra- and inter- self-diffusion coefficients of the aroma in the sol-gel particles were measured in the presence of ethanol. The results were subsequently used to model the release of the aroma measured using UV spectroscopy techniques. [2]

### **3. Conclusion**

In this work we show that self-diffusion experiments can be performed on porous media under magic angle spinning conditions. Both model and real systems were used and the limits of the experiment explored. The data obtained on real systems was successfully applied in models of the release kinetics of aroma from the particles.

### **References**

- [1] S. R. Veith, S. E. Pratsinis, Perren M, Journal of Agricultural and Food Chemistry 52(19),(2004) 5964-5971.
- [2] S. R. Veith, Hughes, E, S. E. Pratsinis, Journal of Controlled Release, 99(2), (2004) 315-327.