Rheological NMR to study polymer dynamics and protein aggregation

B. Kohn[1],V. Körber[1], E. Stündel[1], E. Walinda[2], K. Sugase[3], D. Morimoto[3], P. Galvosas[4], U. Scheler[1]

[1]Leibniz-Institut für Polymerforschung Dresden e.V, Dresden, Germany, [2] Department of Molecular and Cellular Physiology Kyoto University, Kyoto, Japan, [3] Department of Molecular Engineering, Kyoto University, Kyoto, Japan, [4]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand

Introduction: Rheo NMR has been applied to investigate the effect of external shear on the aggregation of proteins [1-2] and on the chain dynamics of polymers [3], where under shear enhanced polymer dynamics is observed instead of shear-induced chain ordering. Most commonly a Couette geometry is applied for such studies. To get further insight two modifications of this are investigated here, where (i) the rotating part in the Couette cell is placed off center and (ii) apply oscillating rotation instead of continuous rotation as applied usually [4].

Methods: Experimenst have been performed on a 300 MHz Bruker AvanceIII spectrometer with a Micro2.5 microimaging accessory and an in-house built rheo NMR system based on a servo motor , avoiding any vibrations. For the oscillatory shear a crank mechanism has been introduced between the motor and the drive of the Couette rotor.

Results and Discussion: Measuring the flow profiles is crucial in both modifications discussed above. In particular for low-viscosity liquids like dilute solutions or lower molecular weight polymers flow pattern deviating from the expected linear velocity gradient are observed. Around the turning point in the oscillatory shear counterflow is observed which leads locally to a shear rate larger than the gap averaged shear rate applied when the angular velocity is at its peak value. For a rotor off the center a counter rotating flow is seen as well in the wider part of the cell.

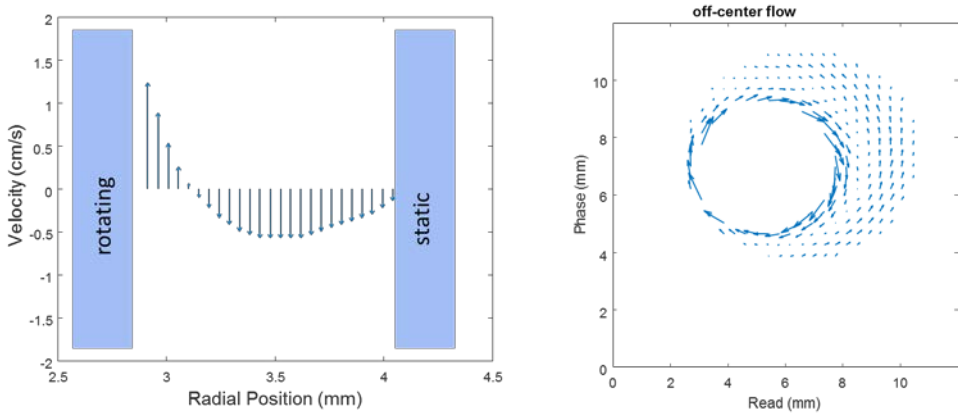

Figure 1: Flow profiles measured combining PFG NMR with imaging. Left: radial flow profile in oscillatory motion in a centered coquette cell just after the turning point exhibiting the counterflow. Right: Two-dimensional flow profile for the cell with the rotor off centered.

Conclusions: Rheo NMR proving very detailed insight in the molecular response to external shear. In addition NMR imaging enables measuring flow profiles in the exact system applied for the investigation of molecular parameters, which is crucial for the interpretation of shear effects in a more complex experimental setup.

References: [1] Ohgo et.al. JACS (2008). [2] Morimoto et. al., Analytical Chemistry (2017). [3] Kohn et. al. Polymer(2018) [4] Kuczera et. al., Langmuir, 2018