CECAM Workshop on "Structure and Rheology of Self-Assembling and Aggregating Colloidal Suspensions: Theory, Simulation and Experiment"

October 12 – 14, 2005
Lyon, France

This workshop was held from 12–14 October 2005 at CECAM (Centre Européen de Calcul Atomique et Moléculaire) and was organized by Edo Boek and Johan Padding. CECAM is based in Lyon and aims at facilitating dissemination and networking activities in the area of computer simulation. For example, 20-25 workshops are being organised at CECAM each year on the subject of particulate computer simulations (see http://www.cecam.fr). The subject of our workshop was to study the link between the structure and rheology of self-assembling and aggregating colloidal suspensions. This is a topic of great importance from both an academic and applied industrial point of view. Significant progress in the design and development of colloidal fluids could be made if a fundamental understanding of the relationship between structure at the molecular / mesoscopic level on the one hand, and the transport and rheological properties on the other hand is achieved. Advancing this understanding was the main objective of our workshop. As main examples, we used the rheology of 1) surfactants self-assembling into wormlike micelles and 2) aggregating colloidal suspensions such as asphaltenes and caseins. Both examples are of great relevance, not only from a fundamental point of view, but also to practical industrial applications.

The workshop had 25 participants from both academic and industrial research institutions (see Fig. 1). The first day started with a session on wormlike micelles, introduced at a fundamental level by Peter Olmsted [1] followed by an outline of industrial applications and simulations [2]. This was followed by a session on rodlike systems and membranes. The second day had sessions on wormlike micelles, colloid simulation and modeling and flow in porous media. The final day had one session on aggregating colloids, with applications varying from caseins to asphaltenes. Finally, many participants took the opportunity to sample the "cuisine lyonnaise" (see Fig. 2).

The picture that emerged from the workshop was that closed form constitutive equations will not give full quantitative predictions for entangled wormlike micellar fluids [3], very similar to the case of entangled polymeric fluids [4]. Coarse-grained modelling tries to balance computational effort with accurate quantitative predictions in agreement with experimental findings. For a full list of participants and abstracts of the workshop contributions, the reader is referred to the CECAM website: http://www.cecam.fr/ (section: past workshops).

To summarise the meeting, we give the conclusions and recommendations resulting from the final discussions:

Figure 1 (left): The workshop participants at CECAM.

Figure 2: Workshop participants sampling the cuisine lyonnaise.

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CONCLUSIONS:

- Self-assembling and aggregating colloidal suspensions, such as wormlike micellar fluids, display a wide range of very interesting rheological phenomena, which are only partly understood.
- The rheological complexity is closely related to the molecular and mesoscopic structure of the colloidal building blocks, but the relationship is not clear in many cases.
- A fundamental understanding of this rheological behaviour is of crucial importance to many industrial applications but is often lacking. This lack of understanding often leads to a very cost-ineffective empirical approach to the design of new responsive fluids.
- The rheological behaviour of wormlike micellar fluids is particularly interesting and only partially understood; the currently available Rheological Equations of State (REoS) only partially explains transient behaviour, normal stresses, extensional viscosity and shear banding instabilities [3]. This may be due to the available REoS being based on phenomenological or heuristic arguments, rather than on a solid microscopic foundation.
- Colloidal asphaltene aggregation in the bulk and its deposition in porous media is of fundamental importance to the oil industry but its foundations are poorly understood.
- The understanding of the flow of complex, non-Newtonian fluids in porous media is even less well developed than that of the bulk flow of such fluids.

RECOMMENDATIONS:

- In order to be able to optimise the rheological behaviour of industrially relevant soft condensed matter systems, the advance of fundamental microscopic understanding of such systems is of crucial importance.
- This advance can only be achieved through a fundamental research effort, combining theory, experiment and simulation.
- More research needs to be done to understand the rheology of wormlike micellar fluids, with the aim to develop a satisfactory REoS. In order to be able to predict the rheological behaviour, the new REoS needs to be based on a microscopic understanding of wormlike micellar fluids.
- The understanding of the flow of complex, non-Newtonian fluids in porous media needs to be developed, for fundamental research and its applications.
- We need a follow-up CECAM workshop to evaluate the progress made in this area. This needs to be done on a time scale of 2-3 years, when a significant advance in the fundamental understanding of wormlike micellar fluids may be expected.

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