Polymers in Fluid Dynamics Problems
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Conclusions & Outlook

In this thesis the mesoscopic simulation method Dissipative Particle Dynamics has been successfully used to model fluid dynamics problems in which polymers play an important role. Especially the influence of polymeric behaviour of solids melting in shear flow has been investigated in detail.

6.1 Boundary conditions

Although the DPD method has been used successfully in unconfined systems, to simulate bulk behaviour, few studies have focused on the presence of a real wall as a boundary to the system. However, such a boundary is obviously a crucial ingredient of flow simulators, like Computational Fluid Dynamics codes. It turned out that implementing a constant temperature boundary condition (Chapter 2) or a constant velocity boundary condition (Chapter 3) is less trivial than it first appears. In grid based discretisations of the governing equations, such as finite difference or
finite element formulation, the implementation of boundary conditions is usually straightforward. A constant temperature is applied by keeping the boundary grid points at this temperature. In an off-lattice method, like DPD, all particles interact with other particles in their interaction radius. This implies that a boundary cannot be represented by a line of points, but should also have the thickness of this interaction radius. In earlier work, researchers have given all the particles that are part of this boundary a constant temperature or velocity. However, when using this implementation, the desired boundary condition was not met. To overcome this error, in Chapter 2 the temperature of these boundary particles is given a slope instead of a constant value. In this way a correct boundary condition is achieved.

The situation for a no-slip condition in velocity can also be solved in this manner, which is described in Chapter 3. In this chapter an additional problem is solved. An undesirable aspect of former boundary condition implementations is the occurrence of density distortions near solid walls. These are caused by elevated wall densities that were used to ensure a no-slip condition. The repulsive interaction present in the DPD scheme will force the particles away from the wall, leading to a low density region at that point. However, when using the newly developed boundary condition method, the density fluctuations become almost negligible.

### 6.2 Melting model

By assigning an energy variable and a temperature to every particle in the DPD scheme, an energy conserving form has been created. In Chapter 2 this approach was used to simulate the phase change of materials. This required the definition of a new equation of state, linking the energy of the material to the temperature in such a way that the enthalpy of fusion can be incorporated as well. In this chapter the new DPD model was tested against analytical solutions of a phase change problem and excellent agreement was found.
6.3 Validation

In addition to these validations of the melting model, the calculated flow fields were compared with other solutions. In Chapter 3 the flow inside a lid-driven cavity was calculated with both DPD and a commercial CFD code, yielding perfect agreement. In Chapter 4 the analytical solution of pressure driven flow in a rectangular cavity was compared with the results of the DPD calculation, again showing very good agreement to CFD.

In both cases mentioned, a solution to the problem could be found with other methods. However, when melting polymers (as performed in Chapter 5), no such solution exists. Therefore, a method to check the simulation results within the DPD method is described in that chapter. This basically comes down to keeping the physical problem the same, while changing the system size of the simulation box. In fact, this changes the resolution of the method and turns out to be a good test of the accuracy of the simulation results.

6.4 Polymers in fluid dynamics problems

6.4.1 Hydrodynamic chromatography

When polymers flow inside small capillaries, the size of the polymer molecule determines the average distance of the centre of mass of this polymer from the walls of the capillary. This will cause large polymers to flow faster though the capillary than smaller polymers, and thus a way of separating polymers of different lengths becomes possible. In Chapter 4 this system was simulated using DPD. It was found that large polymers indeed move at larger distances from the walls of the capillary, which results in a larger mean axial velocity. Thus, the simulation of these systems is feasible with DPD.
6.4.2 Melting in shear flow

The influence of molecular make up on the melting behaviour of a solid object in shear flow is described in Chapter 6. It was found that a solid consisting of connected DPD particles melts more slowly than one consisting of unconnected particles. This increase in melting time is enhanced even further if thermodynamic properties of the polymer are incorporated in the model. If the polymer is less soluble in the fluid, the polymers tend to stick together, even though they are molten and free to move. This decreases the heat flow to the solid, and thus melting progresses is even slower. This shows that DPD is capable of simulating a phase change problem with fluid flow involving polymeric substances. It should be realised that this is difficult, if not impossible with conventional CFD methods.

6.5 Outlook

In this thesis it was shown that DPD is a valuable tool when studying fluid flow problems involving polymers. This thesis has created a foundation for further investigations into this field. Once the problem of boundary conditions has been solved, other issues should be considered in order to render DPD a competitive flow simulator:

- A major disadvantage of DPD is the fact that macroscopic fluid properties are difficult (if not impossible) to predict, given the DPD parameters. In order to upgrade the existing method to a more mature flow simulator, a more thorough understanding of this problem is required.
- An advantage of conventional CFD is the option to use mesh refinement in areas where interesting phenomena take place and coarse meshes in 'smooth' areas. A way to implement this within the DPD scope has to be found. We envision an adaptive coarse/fine graining of DPD particles when needed. This is by no means a trivial task, but it should be tackled.
• In this thesis moderate Reynolds and Peclet numbers have been simulated. A detailed study is required in areas of more extreme values, where the method fails to give correct results.

• An issue in modelling polymer melts remains the handling of entanglements. It is not clear if DPD can or cannot capture this phenomena. The soft repulsions and relatively large time step could result in underestimation of this phenomenon. Perhaps an extra constraint could be added to the DPD scheme, or an adaptive time integration scheme could be implemented when polymers tend to cross each other.

• Finally, an interesting addition to the simulation of polymer melting in shear flow would be to let the solid move with the flow instead of keeping it steady as has been done in this thesis. The solid object is likely to start rotating differently for the various systems that have been studied here. This could lead to some interesting effects on the melting behaviour.


The influence of molecular mass on the melting behaviour of a solid object in shear flow is described in Chapter 6. It was found that a solid consisting of constrained chains exhibits a more smeared out melting point compared to the liquid state. As the molecular mass increases, the melting point also increases, leading to a transition from a glassy state to a more rubbery state. The increase in melting point is even more pronounced in glassy polymers, where the entanglement properties of the chains are not as well expressed as in the liquid state. The polymers tend to stack together even though they are piled up and shear under homologous or homoatomic chain segments, but rubbery polymers remain miscible even if piled up as well. This indicates that DPD is capable of simulating a range of problems involving polymers, which is a significant achievement. In this conclusion, we have demonstrated the versatility of DPD in modeling complex fluid systems and provided insights into the behavior of polymers under various conditions.

6.5 Outlook

In this thesis, we have shown that DPD is a valuable tool when studying fluid flow problems involving polymers. This thesis has created a foundation for further investigations into this field. To solve the problem of boundary conditions, other issues should be considered in order to simulate DPD's competitive flow simulator.

- A major disadvantage of DPD is the fact that mesoscopic fluid properties are difficult (if not impossible) to predict, given the DPD parameters. In order to upgrade the existing method to a more mature flow simulator, a more thorough understanding of this problem is required.

- An advantage of conventional CFD is the option to use mesh refinement in areas where interesting phenomena take place and coarse meshes in smooth areas. A way to implement this within the DPD scope has to be found. We envision an adaptive coarse/fine graining of DPD particles when needed. This is by no means a trivial task, but it should be tackled.