

SIMULATING FLUID FLOW AND HEAT TRANSFER USING DISSIPATIVE PARTICLE DYNAMICS

Erik Johansson

Department of Energy Sciences, Faculty of Engineering
Lund University, Box 118 22100 Lund Sweden
email: erik.johansson@energy.lth.se

ABSTRACT

Dissipative particle dynamics is a relatively new technique for simulating fluid flow at meso scales that is more computationally efficient but at the same time able to reproduce some of the detail of molecular dynamics simulations. This report gives an introduction to the background of the technique, along with examples of applications in the fields of microfluidics, hydrodynamic behaviour at meso scale, and heat transfer. It is shown that dissipative particle dynamics is able to reproduce hydrodynamic behaviour as well as solve simple heat transfer problems. The technique has a large potential to be used in applications where fluid flow is taking place on meso scale where conventional computational fluid dynamics might not be a suitable choice. Two examples of simulations following the approaches of references given in the open literature related to hydrodynamics are also given.

Greek letters

α	Maximum repulsion between particles
β	Repulsion strength in MDPD
γ	Drag coefficient
ρ	Density
$\bar{\rho}$	Average density for MDPD calculations
τ	Stress tensor
σ	Strength of random forces
ζ	Random number
ω	Switching function
ν	Viscosity

Abbreviations

DPD	Dissipative particle dynamics
DPDE	DPD with energy conservation
MDPD	Multibody DPD
Re	Reynolds number
Sc	Schmidt number

Superscripts

C	Conservative
C_m	MDPD Switching function
D	Dissipative
E	Energy

Nomenclature

Latin letters

C_v	Heat Capacity
D	Diffusion
\vec{e}	unit vector
f	Force
m	Mass of DPD particle
q	Heat flux
r	Radius
t	Time
T	Temperature
\vec{v}	Velocity

R Random

Subscripts

i, j	Index
ij	In the direction from i to j
internal	Internal forces
external	External forces
c	Cutoff
d	Many-body cutoff
l, s	Liquid, Surface

Introduction

There are many engineering applications where fluid flow on micro- or nano scales are of importance. Most current efforts on microfluidics concern applications in chemistry, biology and medicine, but there are also applications in the physical sciences such as heat management, energy generation and display technology[1]. Studying microfluidics can also be of great importance for understanding phenomena occurring at nanoliter scale in larger devices, such as electro-chemically active areas of fuel cells[2].

Continuum approach based on solving the Navier-Stokes equations might not be suitable to model fluid flow at mesoscale (micro and nano scales). At the same time, going down to molecular scale and modeling the system using molecular dynamics (MD) is very computationally demanding, and even with the rapid increase in computational power this technique will most probably not be a realistic option in the foreseeable future. Dissipative particle dynamics (DPD) is one possible way of bridging the gap between purely molecular and continuum level treatments[3]. The DPD method is attractive for complex flow simulations, because it does not need a grid for space discretization, and provides correct hydrodynamic macroscale behaviour.

DPD was first introduced by Hoogerbrugge and Koelman [3], and after some minor changes[4], their algorithm is still used today. The method works by grouping fluid molecules together into larger beads. Every bead has a mass localized at one specific point. The beads are deformable and the interactions between them are soft, meaning that particles can pass by or even through each other with relative ease in order to quickly reach equilibrium. For every time step of a DPD simulation three different types of internal interactions occur: conservative repulsion due to the spatial arrangement and energetic interaction between different beads, dissipative interaction due to energy lost due to friction or viscosity within a bead, and a random interaction stemming from the thermal motion of the molecules within the bead. These interactions are taken for every pair of beads within a given range, so called cutoff radius, away from each other. Fig.

1 shows a schematic view of how particles are interacting with each other in a DPD system.

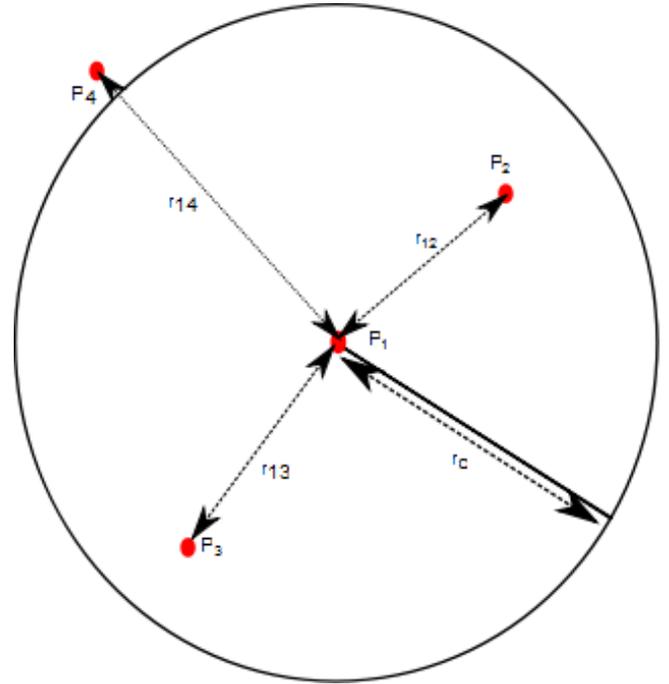


FIGURE 1. Schematic of the interactions of the particle P_1 in a DPD system: particles P_2 and P_3 are located within the cutoff radius r_c and will interact with P_1 , while P_4 is located outside of the cutoff radius and will be ignored

The DPD technique has been used in the fields of biology and chemistry, to study how DNA molecules behave in the flow of a microchannel[5], and the spontaneous vesicle formation of amphiphilic molecules in aqueous solution [6]. Electrostatics have also been employed with DPD to investigate the formation of polyelectrolyte-surfactant aggregates[7]. DPD has gotten attention in simulation of microfluidic flows, for applications such as micropumps[8]. It has also been shown that DPD can be used to simulate fluid flow with good accuracy, even when the Reynolds number of the simulation is as large as 100, and inertia effects are highly involved. This has been shown by different research groups investigating flow around spheres and cylinders [9] as well as in converging-diverging nozzles [10]. Energy is not conserved in the original formulation of the DPD method, making heat transfer impossible to simulate. However, Español [11] proposed a modification to the original DPD method to include new variables for internal energy, entropy and temperature called DPD with energy conservation (DPDe, sometimes also called eDPD). So far, mostly benchmark cases of heat transfer problems with well known solutions have been investigated to

validate the model, but real applications are starting to emerge in the open literature.

Problem Statement

DPD is a promising technique for simulations of fluid flow at nanoliter scale. In order to evaluate how this technique can be used, it is important to look at what has already been done in order to know how it can be possible to move forward. The purpose of this report is to give a background to the theory behind the DPD technique, and review some of the works that have been carried out using DPD to simulate fluid flow, hydrodynamics and heat transfer problems. Calculations done on hydrodynamics are presented, along with ideas on how to incorporate the DPD technique into the modeling of multiphase flows in fuel cell catalyst layers.

Litterature Survey

The litterature survey is divided into two parts. First, the mathematics behind DPD is presented, highlighting the basics of the technique along with the modifications of energy conservation and many-body systems as well as some points on the Schmidt number, which is a debated topic in the field of dissipative particle dynamics. Second, examples of applications for regular DPD, DPD with energy conservation (which might be the most interesting for this course) and many-body DPD is shown.

Mathematical description

The purpose of DPD is to make particle interactions as simple as possible, while still describing the physics of the system in an accurate way. A DPD simulation consists of particles lumped together into beads interacting pairwise with each other according to simplified force laws, and moving according to Newton's second law of motion. The interactions vanish smoothly when the distance between to particles exceed a cutoff radius, r_c . External forces can also be applied to the system. The purpose of this section is to show the general mathematical description of a DPD system. Since the introduction of this technique, several modifications to it have been suggested. In this literature survey, the ideas behind multibody DPD (MDPD) and DPD with energy conservation (DPDe) will also be presented.

The time evolution of the system is given by[12]

$$m_i \frac{d\vec{v}_i}{dt} = (\vec{f}_i)_{internal} + (\vec{f}_i)_{external} \quad (1)$$

where $(\vec{f}_i)_{external}$ is the external force applied to each particle. The internal forces are given by:

$$(\vec{f}_i)_{internal} = \sum_{j \neq i} (\vec{f}_{ij}^C + \vec{f}_{ij}^D + \vec{f}_{ij}^R) \quad (2)$$

where \vec{f}_{ij}^C , \vec{f}_{ij}^D and \vec{f}_{ij}^R are the conservative, drag, and random forces respectively. The index ij means the force exerted on particle i from the particle j . The conservative forces are usually derived from a soft or weakly interacting potential.

The three aforementioned forces are given by:

$$\vec{f}_{ij}^C = \alpha \omega^C(r_{ij}) \vec{e}_{ij} \quad (3)$$

$$\vec{f}_{ij}^D = -\gamma \omega^D(r_{ij}) (\vec{e}_{ij} \cdot \vec{v}_{ij}) \vec{e}_{ij} \quad (4)$$

$$\vec{f}_{ij}^R = \sigma \omega^R(r_{ij}) \zeta_{ij} \Delta t^{-\frac{1}{2}} \vec{e}_{ij} \quad (5)$$

where r_{ij} is the distance between particles i and j , and \vec{e}_{ij} is a unit vector in the direction between particles i and j :

$$\vec{e}_{ij} = \frac{\vec{r}_{ij}}{|\vec{r}_{ij}|} \quad (6)$$

and α is the maximum repulsion between two particles, the constant σ is related to the temperature and gives information about the strength of the random forces, ζ is a random number with zero mean and unit variance, related to the random forces, γ is the drag coefficient, which decides the strength of the dissipative forces, and ω^C , ω^D , and ω^R are the switching functions, ensuring that the interactions between particles vanish smoothly when their distance exceeds the aforementioned cutoff radius. In order for thermodynamic equilibrium to follow from this method, the following relations must be valid[12]:

$$\sigma_{ij}^2 = 2\gamma_{ij} k_B T \quad (7a)$$

$$\omega^D(\vec{r}_{ij}) = (\omega^R(\vec{r})) \quad (7b)$$

and the switching functions can be written as:

$$\omega^C(\vec{r}_{ij}) = \begin{cases} \left(1 - \frac{\vec{r}_{ij}}{r_c}\right), & (\vec{r}_{ij} < r_c) \\ 0, & (\vec{r}_{ij} \geq r_c) \end{cases} \quad (8a)$$

$$\omega^D(\vec{r}_{ij}) = (\omega^D(\vec{r}_{ij}))^2 = \begin{cases} \left(1 - \frac{\vec{r}_{ij}}{r_c}\right)^2, & (\vec{r}_{ij} < r_c) \\ 0, & (\vec{r}_{ij} \geq r_c) \end{cases} \quad (8b)$$

Multibody DPD In order to create better models of the interface between liquid and vapour, the multibody DPD (MDPD) was introduced. The major change in MDPD as compared to the regular DPD is the introduction of an additional attractive force dependent on the local density of the beads, which is introduced to complement the repulsive force described by eq. (3). The dissipative and random forces are described in the same way as for DPD, but the conservative force (eq. 3) is replaced by the following[13]:

$$\vec{f}_{ij}^C = \alpha \omega^c(r_{ij}) \vec{e}_{ij} + \beta [\bar{\rho}_i + \bar{\rho}_j] \omega^{C_2}(r_{ij}) \vec{e}_{ij} \quad (9)$$

where the first term represents a positive interaction ($\alpha \leq 0$) and the second term represents a repulsive reaction ($\beta \geq 0$). The new weight function ω^{C_m} can be thought of as the additional many-body cutoff function and it has a similar appearance as the first conservative weight function:

$$\omega^{C_m}(r_{ij}) = \begin{cases} 1 - \frac{r_{ij}}{r_d}, & r_{ij} < r_d \\ 0, & r_{ij} \geq r_d \end{cases} \quad (10)$$

where r_d is the cutoff radius for the many body-interactions, chosen with the criterion $r_d < r_c$. In the calculations carried out in the following sections, r_d is chosen to be $r_d = 0.75r_c$ as suggested by ref [13]. $\bar{\rho}_i$ is the average local density of the particle i :

$$\bar{\rho}_i = \sum_{j \neq i} \omega_p(r_{ij}) \quad (11)$$

and another weight function ω_p is introduced, which can be written as:

$$\omega_p(r_{ij}) = \begin{cases} \frac{15}{2\pi r_d^3} \left(1 - \frac{r_{ij}}{r_d}\right)^2, & r_{ij} < r_d \\ 0, & r_{ij} \geq r_d \end{cases} \quad (12)$$

DPD with energy conservation In the previous section it has been shown how momentum can be conserved using DPD. In order to also conserve energy, Español [11] introduced DPD with energy conservation in 1994. In DPDe, the particles in the system also exchange energy over the same cutoff radius as previously seen for the conservation of momentum. The energy equation can be written as:

$$C_v \frac{dT_i}{dt} = q_{ij} \quad (13)$$

where C_v is the heat capacity at constant volume, and q_{ij} is the heat flux between particles i and j . This heat flux can be divided into three parts: viscous heating q_{ij}^{visc} , and change in internal energy due to a temperature difference, q_{ij}^{cond} , and fluctuations due to random heat fluxes q_{ij}^R .

$$q_{ij} = q_{ij}^{visc} + q_{ij}^{cond} + q_{ij}^R \quad (14)$$

The three heat fluxes can be written as, respectively[14]

$$q_{ij}^{visc} = \sum_{j \neq i} \frac{1}{2C_v} [(\omega^E)^2(r_{ij}) \{ \gamma_{ij} (\vec{e}_{ij} \cdot \vec{v}_{ij})^2 - \sigma_{ij}^2 m_i \} \quad (15)$$

$$- \sigma_{ij} \omega^E(r_{ij}) (\vec{e}_{ij} \cdot \vec{v}_{ij}) \zeta_{ij}]$$

$$q_{ij}^{cond} = \sum_{j \neq i} \kappa_{ij} (\omega^E)^2(r_{ij}) \left(\frac{1}{T_i} - \frac{1}{T_j} \right) \quad (16)$$

$$q_{ij}^R = \sum_{j \neq i} \alpha_{ij} \omega^E(r_{ij}) \zeta_{ij}^e \Delta t^{-\frac{1}{2}} \quad (17)$$

where ζ_{ij}^e is a random number with zero mean and unit variance. ζ_{ij}^e values are chosen in pairs, and in order to conserve energy the relation $\zeta_{ij}^e = -\zeta_{ji}^e$ must hold[14]. The switching function $\omega^E(r_{ij})$ is given in a similar fashion as the previous switching functions

$$\omega(r_{ij})^E = \begin{cases} \frac{5}{\pi} \left(1 + 3 \frac{r_{ij}}{r_c}\right) \left(1 - \frac{r_{ij}}{r_c}\right)^3, & (\vec{r}_{ij} < r_c) \\ 0, & (\vec{r}_{ij} \geq r_c) \end{cases} \quad (18)$$

Transport Coefficients of a DPD fluid A challenge of the DPD technique is to obtain Schmidt numbers of the correct order of magnitude for liquids. The kinematic viscosity ν and the self diffusion coefficient D can be obtained from using the expressions for drag and stochastic forces[12, 15], and the Schmidt number is then taken defined as the quota between the two: $Sc = \nu/D$:

$$v \approx \frac{45k_B T}{4\pi\gamma\rho r_c^3} + \frac{2\pi\gamma\rho r_c^5}{1575} \quad (19)$$

$$D \approx \frac{45k_B T}{2\pi\gamma\rho r_c^3} \quad (20)$$

$$Sc \approx \frac{1}{2} + \frac{(2\pi\gamma\rho r_c^4)^2}{70875k_B T} \quad (21)$$

Using common values for the drag coefficient and the density yields Schmidt numbers on the order of ≈ 1 which is okay for gasses, but too small for liquids, who have a Schmidt number of approximately one thousand. Peters[16] argued that the Schmidt number is looking at self diffusion of individual molecules, and not DPD beads, making it poorly formulated for DPD simulations, and thus a more realistic Schmidt number is not worth the extra CPU power required. Kumar et al.[17] investigated the impact of Schmidt number of the water flow in a microchannel by varying the coarse graining parameter (a measurement of how many particles are included in each bead) and observed that diffusion of a coarse grained particle did not correspond to self diffusion of individual molecules and concluded that the Schmidt number is not an accurately defined parameter for a coarse grained system. Other authors[18] say that the agreement with experiments improve when the value of Sc increases to values closer to what you would expect from a liquid.

Applications of DPD

This section will cover how DPD, MDPD, and DPDe have been used in different applications. The standard DPD method is not suitable for modeling heat transfer problems because of its inability to conserve energy. The applications of DPD are to a large extent related to flow on meso scale, and it is therefore interesting to see how well the model can capture hydrodynamic behaviour at these scales. An example is shown in fig 2[19], where the DPD technique is used to simulate fluid flow in a microchannel system, with phenomena such as tension between surface and liquid adequately matched with experimental data.

Multibody DPD

Modeling the surface tension between liquid water and other fluids is of great importance whenever a good bulk model of liquid water is of importance, such as in modeling fluid flow in microchannels, or in the catalyst layers of fuel cells. The interface tension between liquid water droplets and a surrounding fluid has been investigated using MDPD by Ghoufi and Malfreyt[13]. Fig 3 shows a simulation using their approach carried out using the free software DL_meso2.5[20] with visualization performed by

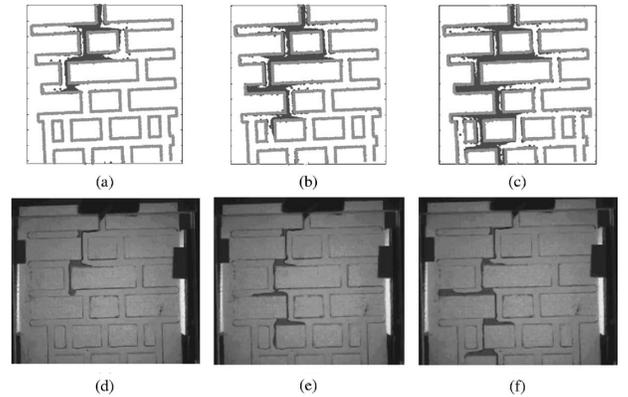


FIGURE 2. Sequential images of fluid flow in a microchannel network: the first three images (a-c) shows DPD simulations, and the last three images shows photographs of an experimental setup at three equivalent stages[19]

the software VMD[21]. In the initial stage, the water beads are evenly distributed in the domain, and at the final timestep the beads have aggregated due to the surface tension between the water bead and the surrounding vapour. The figure shows two different aggregates, one at the far left and one at the far right. This, is however due to the periodic boundary conditions used. The two aggregates should really be thought of as only one.

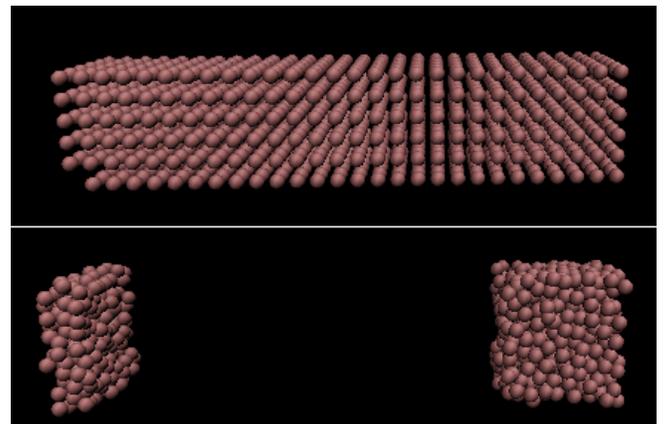


FIGURE 3. liquid-vapour interface simulated using the software DL_Meso2.5: **top)** initial configuration of water particles uniformly distributed in the domain **bottom)** configuration at the last timestep.

The MDPD method has also been used to simulate surface tension between a liquid and a solid [22], displaying that the DPD technique is capable of simulating interactions between fluids and materials with different, and by changing the solid-liquid

attraction parameter A_{sl} , achieve different static contact angles between the solid and the liquid and thus create surfaces with different hydrophobicity.

DPDe with energy conservation

The literature published on DPDe is still rather limited and a lot still needs to be done to validate the technique against benchmark heat transfer problems[23]. The technique has been used to simulate two-dimensional multicomponent flow with heat conduction [24], natural convection problems [23, 25] and forced convection problems [14]. An example of the validation of the DPDe method is given by Yamada et. al[14]¹ and is shown in fig 4. Three sides of a rectangular plate are kept at a constant, cold T_c , temperature, and the fourth wall is kept at a constant, higher T_H , temperature. The dimensionless velocity profile is simulated and compared to the analytical solution given by Incropera and DeWitt[26].

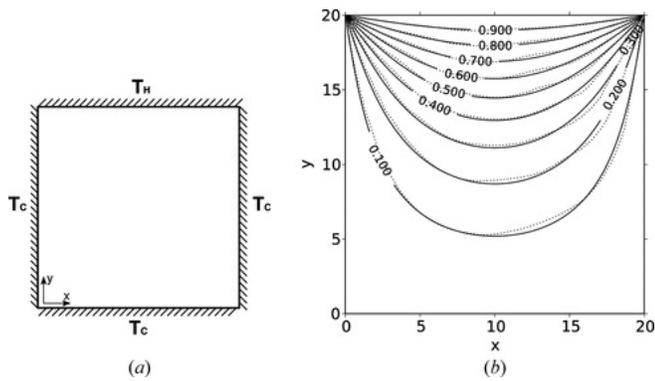


FIGURE 4. Two-dimensional steady heat conduction simulated with DPDe: a) Schematic of the solution domain, b) comparison between analytical and DPDe solution[14]

DPDe has also been used to simulate heat transfer with moving boundaries, as described in chapter two of the text book for this course[27], by introducing the interface conditions between solid and liquid material in a melting process[28]. The evolution of the melting over time is displayed together with the analytical result in fig 5, and an excellent agreement is shown, displaying that DPDe is also capable of simulating systems undergoing phase change.

Applications of the DPDe technique so far include simulation of thermal conductivity of nanofluids [29], and simulation of heat conduction in nanocomposite materials [30]. DPDe has been used to simulate heat conduction problems in one dimen-

¹The author of this work is starting a post-doctoral employment at the department of heat transfer at LTH in September 2012.

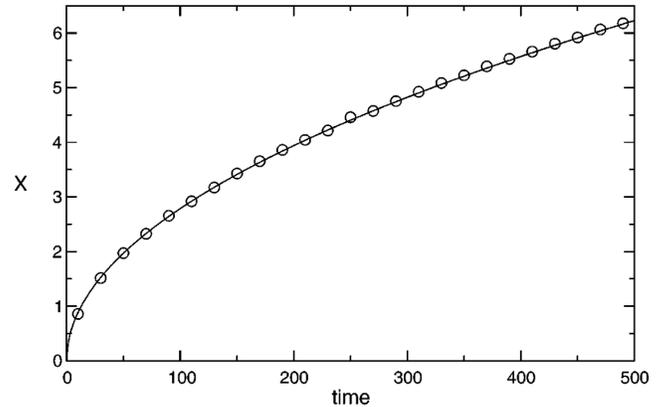


FIGURE 5. DPDe simulation of a melting process, circles are the DPDe simulations, and the solid line represents the analytical solution[28]

sion and two dimensions, but to this author’s knowledge, three-dimensional simulations are yet to be seen.

Project Description

This section gives an example of how DPD can be used to simulate the behaviour of a water droplet forming on a flat plane, and a discussion on how the DPD technique can be implemented in my current research regarding fluid flow in the catalyst layers of proton exchange membrane fuel cells. The water droplet on a flat plate-simulation is relevant, because it can help investigate how the attractive and repulsive parameters α and β in the MDPD simulations can be set to achieve different hydrophobicity for different materials. Another way to investigate hydrophobicity using DPD is to

A rather small simulation box is demonstrated, to show how some of the important ideas covered by the literature review can be incorporated. By following the procedure of ref. [13], water was modelled using the MDPD method with beads consisting of three water molecules each, and the parameters A and B from eq. 9 are set to -40.0 and 25.0 , r_{bead} and r_c are set to unity. The time step Δt is set to 0.01 DPD units, which corresponds to 6.8 picoseconds in real-world units. The method is then modified by including an external gravity force set to 0.02 which is in agreement with ref[19], and applying a solid boundary consisting of frozen beads with the same density and radius as the liquid, and the parameter α set so that $\alpha_{ss} = \alpha_{ll}$, $\alpha_{sl} > \alpha_{ll}$ as suggested by ref [22]. Frozen in this sense means that the position of the particle is frozen, but the interactions with the mobile particles are still weakly interacting, meaning that it is possible for mobile particles to pass through the solids. If this is not desirable, it can be avoided by increasing the density of the frozen particles[31]. 4000 beads are modelled in a domain consisting

of $27.0 \times 14.0 \times 27.0$ DPD length units, corresponding to a real-world volume of 6312 nm^3 . Fig. 6 shows the time evaluation of the system. It can be seen how the fluid molecules aggregate, at first in smaller droplets, and at the final configuration as one droplet located on the solid surface. Running the simulation for 40000 timesteps takes roughly 30 minutes using the software DL_MESO2.5 operating with one processor. It is possible to run the application in parallel in order to increase the computational speed if larger domains are to be modelled.

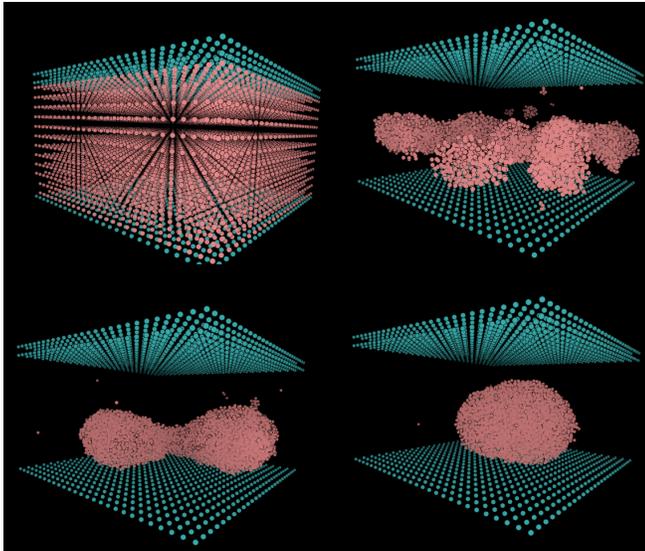


FIGURE 6. Simulation of the formation of a water droplet on a flat hydrophobic surface: a, initial configuration, b, configuration after 1000 time steps, c, configuration after 2000 time steps, d, configuration after 10000 timesteps

This technique can be suitable for simulating fluid flow in nanoscale structures created by coarse grained molecular dynamics, such as the ones already produced by our research group[32]. Since DPD is a meshless technique, and all beads in a simulation has a point mass, it is relatively easy to introduce structural output data from a coarse grained molecular dynamics simulation into a DPD simulation box as frozen particles. The idea would be to recognise the different materials in the domain, and supply them with different attractive and repulsive strengths for the interaction potentials to produce different hydrophobicity in a manner similar to what was suggested in ref [22]. In this way multiphase flow of the structure could be simulated with realistic interaction between the solid material and the fluids. The major challenge is also simulating chemical reactions and phase change. Even though phase change has been shown using DPD as presented in the previous sections implementing it in this kind of system would require a lot of hard work.

Conclusions

This report has covered the basics of dissipative particle dynamics; the underlying mathematics and principal workings, along with a literature review on some of the applications related to heat- and mass transfer with examples of applications already available in the open literature as well as some calculations to reproduce the results of other authors with slight modifications. Ideas on how to use the DPD for simulating fluid flow in a nano-scale reconstruction of a proton exchange membrane fuel cell catalyst layer are presented. It is shown that the DPD method has the potential to reproduce hydrodynamic behaviour of water at meso scale, making the technique suitable for modeling multiphase flows at such length scales, even in irregular domains. It is also shown that the technique is promising in describing heat transfer phenomena, although this field is still in the early stages of its development.

REFERENCES

- [1] Squires, T. M., and Quake, S. R., 2005. "Microfluidics: Fluid physics at the nanoliter scale". *Reviews Of Modern Physics*, **77**, pp. 977–1026.
- [2] Mukherjee, P. P., Kang, Q., and Wang, C.-Y., 2011. "Pore-scale modeling of two-phase transport in polymer electrolyte fuel cells-progress and perspective". *Energy Environ. Sci.*, **4**, pp. 346–369.
- [3] Hoogerbrugge, P. J., and Koelman, J. M. V. A., 1992. "Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics". *EPL (Europhysics Letters)*, **19**(3), p. 155.
- [4] Espanol, P., and Warren, P., 1995. "Statistical mechanics of dissipative particle dynamics". *EPL (Europhysics Letters)*, **30**(4), p. 191.
- [5] Fan, X., Phan-Thien, N., Yong, N. T., Wu, X., and Xu, D., 2003. "Microchannel flow of a macromolecular suspension". *Physics of Fluids*, **15**(1), pp. 11–21.
- [6] Yamamoto, S., Maruyama, Y., and aki Hyodo, S., 2002. "Dissipative particle dynamics study of spontaneous vesicle formation of amphiphilic molecules". *The Journal of Chemical Physics*, **116**(13), pp. 5842–5849.
- [7] Groot, R. D., 2000. "Mesoscopic simulation of polymer surfactant aggregation". *Langmuir*, **16**(19), pp. 7493–7502.
- [8] Palma, P. D., Valentini, P., and Napolitano, M., 2006. "Dissipative particle dynamics simulation of a colloidal micropump". *Physics of Fluids*, **18**(2), p. 027103.
- [9] Kim, J. M., and Phillips, R. J., 2004. "Dissipative particle dynamics simulation of flow around spheres and cylinders at finite reynolds numbers". *Chemical Engineering Science*, **59**(20), pp. 4155 – 4168.
- [10] Abu-Nada, E., Kumar, A., Asako, Y., and Faghri, M., 2012. "Dissipative particle dynamics for complex geometries us-

- ing non-orthogonal transformation”. *International Journal for Numerical Methods in Fluids*, **68**(3), pp. 324–340.
- [11] Espanol, P., 1997. “Dissipative particle dynamics with energy conservation”. *EPL (Europhysics Letters)*, **40**(6), p. 631.
- [12] Groot, R. D., and Warren, P. B., 1997. “Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation”. *The Journal of Chemical Physics*, **107**(11), pp. 4423–4435.
- [13] Ghoufi, A., and Malfreyt, P., 2011. “Mesoscale modeling of the water liquid-vapor interface: A surface tension calculation”. *Phys. Rev. E*, **83**, May, p. 051601.
- [14] Yamada, T., Kumar, A., Asako, Y., Gregory, O. J., and Faghri, M., 2011. “Forced convection heat transfer simulation using dissipative particle dynamics”. *Numerical Heat Transfer, Part A: Applications*, **60**(8), pp. 651–665.
- [15] Marsh, C. A., Backx, G., and Ernst, M. H., 1997. “Static and dynamic properties of dissipative particle dynamics”. *Phys. Rev. E*, **56**, Aug, pp. 1676–1691.
- [16] Peters, E. A. J. F., 2004. “Elimination of time step effects in dpd”. *EPL (Europhysics Letters)*, **66**(3), p. 311.
- [17] Kumar, A., Asako, Y., Abu-Nada, E., Krafczyk, M., and Faghri, M., 2009. “From dissipative particle dynamics scales to physical scales: a coarse-graining study for water flow in microchannel”. *Microfluidics and Nanofluidics*, **7**, pp. 467–477. 10.1007/s10404-008-0398-x.
- [18] Symeonidis, V., Karniadakis, G. E., and Caswell, B., 2006. “Schmidt number effects in dissipative particle dynamics simulation of polymers”. *The Journal of Chemical Physics*, **125**, pp. 184902–1–184902–12.
- [19] Liu, M., Meakin, P., and Huang, H., 2007. “Dissipative particle dynamics simulation of multiphase fluid flow in microchannels and microchannel networks”. *Physics of Fluids*, **19**(3), p. 033302.
- [20] Seaton, M. A., 2012. *The DL-MESO Mesoscale Simulation Package*. STFC Computational Science and Engineering Department.
- [21] Humphrey, W., Dalke, A., and Schulten, K., 1996. “Vmd - visual molecular dynamics”. *J. Molec. Graphics*, **14**, pp. 33–38.
- [22] Cupelli, C., Henrich, B., Glatzel, T., Zengerle, R., Moseler, M., and Santer, M., 2008. “Dynamic capillary wetting studied with dissipative particle dynamics”. *New Journal of Physics*, **10**(4), p. 043009.
- [23] Abu-Nada, E., 2011. “Application of dissipative particle dynamics to natural convection in differentially heated enclosures”. *Molecular Simulation*, **37**(2), pp. 135–152.
- [24] Chaudhri, A., and Lukes, J. R., 2009. “Multicomponent energy conserving dissipative particle dynamics: A general framework for mesoscopic heat transfer applications”. *Journal of Heat Transfer*, **131**(3), p. 033108.
- [25] D. Mackie, A., Bonet Avalos, J., and Navas, V., 1999. “Dissipative particle dynamics with energy conservation: Modelling of heat flow”. *Phys. Chem. Chem. Phys.*, **1**, pp. 2039–2049.
- [26] Incropera, F. P., and DeWitt, D. P., 1981. *Fundamentals of Heat Transfer*. John Wiley & Sons, Inc.
- [27] Sunden, B., and Yuan, J., 2012. *MVK 160 Heat and Mass Transfer*. Energivetenskaper.
- [28] Willemsen, S., Hoefsloot, H., Visser, D., Hamersma, P., and Iedema, P., 2000. “Modelling phase change with dissipative particle dynamics using a consistent boundary condition”. *Journal of Computational Physics*, **162**(2), pp. 385 – 394.
- [29] Yamada, T., Asako, Y., Gregory, O. J., and Faghri, M., 2012. “Simulation of thermal conductivity of nanofluids using dissipative particle dynamics”. *Numerical Heat Transfer, Part A: Applications*, **61**(5), pp. 323–337.
- [30] Qiao, R., and He, P., 2007. “Simulation of heat conduction in nanocomposite using energy-conserving dissipative particle dynamics”. *Molecular Simulation*, **33**(8), pp. 677–683.
- [31] Pivkin, I. V., and Karniadakis, G. E., 2005. “A new method to impose no-slip boundary conditions in dissipative particle dynamics”. *Journal of Computational Physics*, **207**(1), pp. 114 – 128.
- [32] Xiao, Y., Dou, M., Yuan, J., Hou, M., Song, W., and Sundén, B., 2012. “Fabrication process simulation of a pem fuel cell catalyst layer and its microscopic structure characteristics”. *Journal of The Electrochemical Society*, **159**(3), pp. B308–B314.