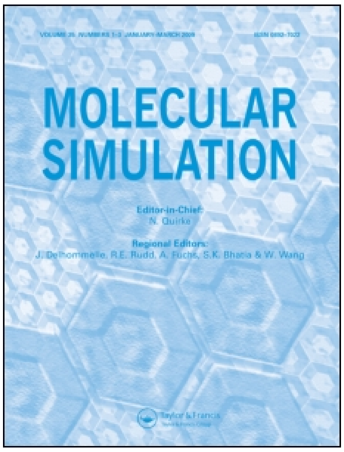

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Simulation of Suspensions in Constricted Geometries by Dissipative Particle Dynamics

J. R. Darias[a]; M. Quiroga[a]; E. Medina[a]; P. J. Colmenares[b]; R. Paredes[a]
[a] Laboratorio de Física Estadística de Sistemas Desordenados, Centro de Física, IVIC, Caracas, Venezuela [b] Departamento de Química, Núcleo La Hechicera, Universidad de los Andes, Mérida, Venezuela

Online publication date: 26 October 2010

To cite this Article Darias, J. R. , Quiroga, M. , Medina, E. , Colmenares, P. J. and Paredes, R.(2003) 'Simulation of Suspensions in Constricted Geometries by Dissipative Particle Dynamics', Molecular Simulation, 29: 6, 443 — 449
To link to this Article: DOI: 10.1080/0892702031000148753
URL: http://dx.doi.org/10.1080/0892702031000148753

Molecular Simulation, Vol. 29 (6–7), June 2003, pp. 443–449

Taylor & Francis
Taylor & Francis Group

Simulation of Suspensions in Constricted Geometries by Dissipative Particle Dynamics

J.R. DARIAS[a], M. QUIROGA[a], E. MEDINA[a,*], P.J. COLMENARES[b] and R. PAREDES V[a]

[a]*Laboratorio de Física Estadística de Sistemas Desordenados, Centro de Física, IVIC, Apartado 21827 Caracas 1020A, Venezuela*
[b]*Departamento de Química, Universidad de los Andes, Núcleo La Hechicera, Mérida 5101, Venezuela*

(Received November 2002; In final form February 2003)

We investigate the flow of a suspension through a constriction by means of the mesoscopic technique known as dissipative particle dynamics (DPD). The dispersed phase was modeled as a set of soft spheres interacting through a conservative force while suspended and continuum phases interact via DPD forces. It is shown that a Poiseuille steady state is achieved in the presence of bounding walls and under a pressure gradient in a cylindrical pipe. Flow geometry in the laminar regime is explored and discussed for periodic conditions in the presence of a cylindrical narrowing or constriction.

Keywords: Suspensions; Constricted geometries; Dissipative particle dynamics; Molecular dynamics

INTRODUCTION

Physically, the description of complex fluid systems by molecular dynamics (MD) faces two mayor problems: one has to do with the correct definition of the interaction potential, and the second, regarding its computational implementation, is the management and control of the relatively large number of degrees of freedom for the system to reach macroscopic behavior. These two factors limit severely the scope of the application of MD and particularly they become unmanageable when the complexity of the system is increased, such as in the flow of emulsions, oils, colloids and other complex fluids through pipes and restricted geometries with complex boundary conditions. In these cases and in order to grasp information about the hydrodynamic behavior of the fluid, it is customary to appeal to statistical tools developed in the physics of many particles.

One of the ideas is to reduce the number of degrees of freedom while preserving in the new description the statistical character of the original system. In doing this process, molecular fluctuations appear naturally and therefore, it is necessary to use the theory of stochastic processes for the complete statistical description of the system. This is the essence of any mesoscopic dynamical method; it has the disadvantage that the molecular details of MD are lost due to the process of contraction, but the contraction itself simplifies the problem at lends access to the scales required from the computational point of view.

This point of view, which is amply used in Brownian dynamics (BD), was extended by Hoogerbrugge and Koelman [1,2] to the realm of hydrodynamics. This promising technique, christened Dissipative particle dynamics (DPD), converts an automaton-like algorithm into a molecular dynamic scheme to describe coarse grained hydrodynamics, a level of description absent in conventional diffusive Brownian dynamics. By updating in discrete time steps the interparticle collision step followed by a space propagation, they were able to simulate a 3D flow of particles through a square array of cylinders [1] as well as a soft sphere dispersions under steady shear [2]. Later on, Español and Warren [3] established the theoretical basis of the Hoogerbrugge *et al.*'s original work. They based their analysis on the theory of stochastic differential equations and their corresponding Fokker–Planck formalism, to justify, among other things,

*Corresponding author.

ISSN 0892-7022 print/ISSN 1029-0435 online © 2003 Taylor & Francis Ltd
DOI: 10.1080/0892702031000148753

the existence of a fluctuation–dissipation theorem for this system. It is worth also mentioning the simulations done by Coveney and Novik [4] in the analysis of the dynamics of a 2D binary inmiscible fluid. They monitored phase separation and found the corresponding algebraic laws of growing domains concluding that DPD is a promising method for simulating suspensions. This is convalidated by Groot and Warren [5] who made a critical review of the method, specifically by determining the range of parameters demanded by a real simulation, i.e. the strength of the noise and the magnitude of the timestep.

As we mentioned earlier, one of the mayor problems in simulations is the management of complex boundary conditions and particularly when a suspension is involved. One widely used trick implemented within the DPD method, is to mimic obstacles such as cylinders, spheres, rods and flat walls, and even the suspended particles by using the mesoscopic particles themselves. It consists in freezing some portions of the DPD fluid so that the frozen ensemble acts as either a fixed or a moving boundary [1–8]. This is particularly suitable if the boundary is moving within the fluid, as in the case of a suspension, but has the disadvantage that particles can penetrate the boundary with the subsequent appearance of boundary slip. In order to overcome this issue, it is customary to use the Lees–Edward sliding periodic boundary condition [9], as done by Boek *et al.* [10,11] in their study of the rheology of suspensions or alternatively, by the method designed by Revenga *et al.* [12,13] based on calculating the effective force on the dispersed particles, due to the particles of fluid striking the interface. They found that whenever a particle hits the boundary, a bounce back reflection mechanism produces no-slip boundary conditions for any value of the control parameter.

In this work, we propose to further exploit bounce back boundary conditions to simulate flow of a DPD fluid including suspended particles in the presence of boundary walls in three dimensions. We will also use a combined molecular dynamics approach to describe the suspended phase. Here the dispersed components are represented by larger particles that interact via conservative forces, instead of using the frozen particle schemes described in the literature. Under such conditions we show that the systems achieve the correct isothermal equilibrium conditions, and under a pressure gradient assume the familiar Newtonian flow patterns expected. Finally, we make a preliminary investigation of the effects of a constriction on the resulting flow under periodic boundary flow conditions. The interest on a constriction geometry is that it is the simplest model of what a suspension undergoes in a porous medium. One fundamental issue in secondary oil recovery is the stability of "smart" suspensions injected to remove remaining oil. The modification of the nature of the suspension under strong shear within pore throats can change its properties.

This paper is organized as follows: In the second section we give a brief statistical mechanics foundation of the DPD method, as well as some general remarks about essential numerical considerations. The third section deals with our main results regarding the flow of the suspension through a cylindrical pipe geometry and in the presence of a narrowing or constriction. We end, in the fourth section, with a discussion and conclusions.

THEORY

Because of the contraction of the number of degrees of freedom within a mesoscopic description, the particles in DPD are not fundamental entities as in MD. They represent a cluster of microscopic particles interacting under a given, renormalized force. A set of propagation rules based on these forces change their position and momenta. This coarse graining process leads inevitably to a loss of information and the subsequent appearance of new time and length scales.

In the DPD description, the total force acting on the mesoparticle is split into: (i) a conservative part that accounts for the effect of the two particle interaction potential, (ii) a dissipative term and (iii) a stochastic component. Thus, if the suspension is composed of N interacting mesoparticles, at the temperature T, the equations of motion read

$$\frac{\mathrm{d}\vec{P}_i}{\mathrm{d}t} = \sum_{j \neq i} \left[\vec{F}_{ij}^{\,C} + \vec{F}_{ij}^{\,D} + \vec{F}_{ij}^{\,R} \right], \tag{1}$$

$$\frac{\mathrm{d}\vec{r}_i}{\mathrm{d}t} = \frac{\vec{P}_i}{M}, \tag{2}$$

where $\vec{P}_i$, $\vec{r}_i$ and M are the momentum, position and mass of the mesoparticle, and the supraindexes $\{C, D, R\}$ refer to the conservative, dissipative and random contributions, respectively.

As opposed to Brownian dynamics, where the movement of the particle is eminently diffusive, mesoparticles in DPD propagate in phase space hydrodynamically because in addition to mass, also momentum is conserved. The energy is not conserved in the DPD approach and thus there is a lack of a transport equation for heat conduction [14,15]. Furthermore, because there is no other source of dissipation, such as a temperature gradient to promote a heat transfer, a DPD fluid cannot keep a temperature difference and therefore, the temperature relaxes to a global predetermined value. This behavior contrasts deeply with that found in a Navier–Stokes fluid in which the mass, momentum and energy fields kinetically relax to their local values. In conclusion, in equilibrium conditions (no macroscopic currents present) the kinetic energy relaxes to its equipartition value and, because it depends on the density field, any transport equation for this property leads inexorably to the continuity equation [15].

It was pointed out by Español *et al.* [3], that the expressions for the forces D, R and C in the different applications of this technique are given by

$$\vec{F}_{ij}^{C} = \alpha\omega_C(\vec{r}_{ij})\hat{e}_{ij}, \tag{3}$$

$$\vec{F}_{ij}^{D} = -\gamma\omega_D(\vec{r}_{ij})(\hat{e}_{ij}\cdot\vec{v}_{ij})\hat{e}_{ij}, \tag{4}$$

$$\vec{F}_{ij}^{R} = \sigma\omega_R(\vec{r}_{ij})\zeta_{ij}\hat{e}_{ij}, \tag{5}$$

where $\vec{v}_{ij} = \vec{v}_i - \vec{v}_j$ is the relative velocity of the mesoparticles, $\hat{e}_{ij}$ is a unitary vector pointing from particle i to particle j, α is a parameter of the conservative force defining the compressibility of the fluid and ζ_{ij} is a delta correlated zero mean random Gaussian function

$$\langle\zeta_{ij}(t)\rangle = 0, \tag{6}$$

$$\langle\zeta_{ij}(t)\zeta_{kl}(s)\rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\delta(t-s), \tag{7}$$

where $\omega_{(D,R)}(\vec{r}_{ij})$ is a weight function depending on the relative position vector of the pair of mesoparticles $\vec{r}_{ij}$. Constants γ and σ account for the relative importance of these forces and are related to each other, through a fluctuation dissipation relation to guarantee the equilibrium state at the given T. The stochastic component comes from the fact that at very short times the unpredictability of the movement shows up because in the limit $\Delta t \to 0$, the product $\zeta_{ij}(t)\mathrm{d}t$ changes at a very high rate. Mathematically, this is equivalent to a Wiener process [16], so the random force with the definition (5) can be written as

$$\vec{F}_{i}^{R} = \sum_{j\neq i}\sigma\omega_R(\vec{r}_{ij})\hat{e}_{ij}\mathrm{d}W_{ij}, \tag{8}$$

where $\mathrm{d}W_{ij}$ is the differential increment of the Wiener process.

The equilibrium state of a DPD system was investigated by Español and Warren [3] by recognizing that the two stochastic variables $\vec{r}_i$ and $\vec{P}_i$, have a probability measure described by a bi-variate Fokker–Planck equation (FPE) which can be easily derived from standard techniques of stochastic differential equations [16]. Even though there is no formal solution to it, their argument was based on that any initial measure will necessarily be propagated to a Gibbsian distribution as a condition for the existence of equilibrium [17]. In this context, and working in the framework of the canonical ensemble, they found that in order to attain the equilibrium state, constants ω_R and ω_D must fulfill the requirement

$$\omega_R(r) = \omega_D^{1/2}(r), \tag{9}$$

$$\sigma = (2kT\gamma)^{1/2}. \tag{10}$$

These last two expressions are the dissipation–fluctuation (FD) relations for the DPD method. They limit the intensities of the noise as a function of the energy dissipated by friction, as well as it gives the relation between the function ω_R and ω_D. The choice of the r dependent function $w(r)$ in the three DPD forces is the usual linear function [1] $(1 - r/r_c)$ where r_c is a cutoff distance for the interaction.

SUSPENSION MODEL

We consider a model dispersion as a highly incompressible fluid whose dispersed units are neutrally buoyant. It is composed of a continuous phase of DPD particles, whose cutoff interaction is $r_c = 1$, and a dispersed phase formed by spherical particles of diameter $4r_c$. The mass density of the continuous phase is $\rho_{cp} = Mn$ where n is the number density and M is the mass per DPD particle. The neutral buoyancy condition is fulfilled by equating the density of the continuous phase and that of the dispersed particles. From here we determine that the mass of a suspended particle to be $nM(32/3)\pi r_c^3$.

The forces describing the continuous phase follow those of regular DPD, and are described in Ref. [3]. The intensity of the noise, or equivalently the amplitude of the dissipation according to the fluctuation dissipation theorem, is fixed so as to obtain a given temperature T. The parameter of the conservative force is determined on thermodynamical grounds following the procedure described in Groot *et al.* [5] that fixes the compressibility of the fluid. Regarding the interactions between particles of the dispersed phase, we chose a soft repulsion given by

$$\vec{F}_{ij}^{\mathrm{dp}} = \begin{cases} (\alpha_d/r_c)(4r_c - r_{ij})\hat{e}_{ij} & (r_{ij} < 4r_c) \\ 0 & (r_{ij} \geq 4r_c) \end{cases}, \tag{11}$$

where α is the parameter characterizing the conservative force of the DPD particles [5]. The prefactor α_d parameterizing the forces between dispersed particles was chosen to insure at least the same effective force constant $(\mathrm{d}F^C/\mathrm{d}r_{ij})$ as that between particles of the continuous phase. Nevertheless, in practice α_d was increased further, to a value of 40α, because as the large particles approach each other a net attraction between them arises due to the excluded particles of the continuous phase.

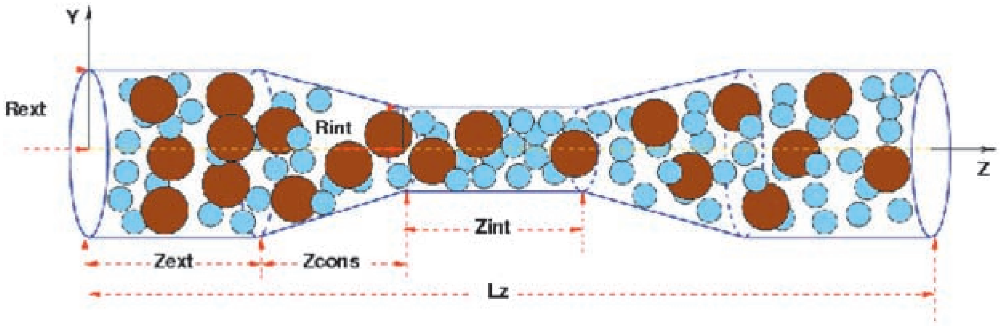

FIGURE 1 Cylindrical geometry. The total length of the system L_z is divided in five sections, included two gradual regions taking the cylinder from the large radius to the constriction radius and vice-versa. The interaction of DPD particles with the surface is modeled using bounce-back boundary condition. (Colour version available online.)

The extra force imposed counteracted such discreteness effect of the fluid.

For the interaction between particles of the continuous and suspended phase we use DPD type interactions as expounded in the previous section and repeat the recipe detailed above only fixing the force constants (with no exclusion effects considered). The cutoff distance for this case, referred to that of the continuous phase, is $5/2\,r_c$. The intensity of the corresponding dissipative force was estimated for this geometry [18] following the method outlined by Revenga *et al.* [12,13] in the determination of the effective force of DPD particles and a wall composed of frozen mesoparticles. Once the dissipative force constant is determined a simple application of the fluctuation dissipation relations using Eq. (10), determines the random force constant.

The flow geometry including the constriction is depicted in Fig. 1. It is axially symmetric around the chosen z-axis. To simulate the flow and to guarantee both, non-slip on the walls and a uniform temperature in their vicinity, a bounce back reflection mechanism was applied to any particle colliding with the boundary [12]. This condition was found to be much better than simulating the wall as frozen particles which results in a excluded volume close to the boundary and wide deviations of temperature in its vicinity.

RESULTS

In this work, the Groot and Warren's modified version [5] of the velocity Verlet algorithm [19] was implemented to perform all the numerical integration of the equations of motion. Before we specialize our calculations to the flow through the constriction, we validate our model with the expected standard hydrodynamic behavior, by determining properties in elemental geometries, such as a cylindrical pipe. In Fig. 2, we show the parabolic velocity profile, $v(r)$, scaled by the pressure gradient ΔP in a cylindrical geometry. The pressure gradient was implemented in our algorithm by adding, in the direction of the flow, a constant external force (linearly proportional to the mass) to the total force exerted on each particle. The data collapse onto the same universal curve when the velocity is scaled by the pressure gradient as expected for Poiseuille flow. The insets show the R^2 and the L_z dependence of the flow prefactors. We can see that all figures, for distances from the wall greater than r_c, collapse to a unique quadratic function of the distance from the fluid bulk. This agrees with Newtonian behavior in which the profile is given by

$$v(r) = \frac{\Delta P R^2}{4\eta L}\left[1 - \left(\frac{r}{R}\right)^2\right], \tag{12}$$

where η is the viscosity of the fluid and R the radius of the pipe. If we keep the pressure gradient constant and vary the pipe length, we can collapse all curves to a single universal function as shown in the inset of

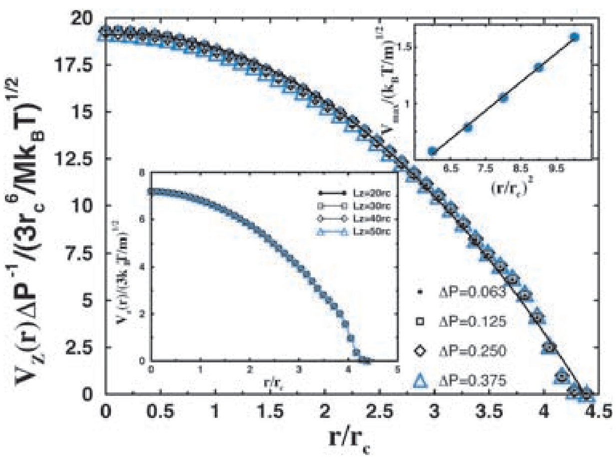

FIGURE 2 Poiseuille collapse for different pressure gradients. These profiles correspond to a monophasic fluid of $N = 3817$ particles, and density $\rho = 3.0\,\mathrm{m}/r_c^3$, in a pipe of length $L = 20\,r_c$ and radius $R = 4.5\,r_c$. The collapse of these profiles indicates that the fluid is Newtonian under the gradients reported. The continuous line shown is a quadratic fit to the data. The lower inset shows a similar collapse fixing the pressure gradient and varying the pipe length. The upper inset demonstrates the quadratic dependence with the pipe radius.

Fig. 2. This collapse is by no means trivial since it implies a shear independent viscosity of the DPD fluid.

We observe from Fig. 2 that at distances very close to the wall, the distribution deviates from a parabolic dependence. The lack of parabolic dependence, at length scales of the order of the DPD cutoff distance from the wall, springs from the discrete nature of the formulation. The discreteness of the system is directly seen by examining Fig. 3 for the density profile. We can clearly see that particles tend to pack in a crystalline-like fashion, in the vicinity of the wall. This edge effect is important for distances of the order of r_c and is of no consequence to bulk behavior.

Subsequently, we included a bottle-neck constriction, as described in the previous section, and checked, using pure DPD fluid under a pressure gradient, for the fulfillment of laminar flow conditions. For PBC along the axis of the pipe it is also necessary to find the appropriate ratio of the total length of the pipe to the length of the constriction, to minimize feedback effects. The length of the pipe was set so that the fluid achieves a Poiseuille velocity profile at the flow exit. An appropriate flow pattern is obtained for a pipe length, after the constriction, equal to twice the total constriction length at the chosen constriction radius (see Fig. 1). We also found that in order to get a Poiseuille profile in the constriction, it is imperative to set its length so as to minimize the effects of the spatial transient due to the change in radius of the pipe. The results are shown in Fig. 4 where the neck length is of $32r_c$. It can be seen that the region before the constriction follows a parabolic dependence (Fig. 4a), while inside the neck the dependence is better fitted by a cubic dependence (Fig.4b). Poiseuille flow can be found by increasing the neck length. In both previous situations (in and out of the constriction), the profile was measured in the vicinity of the center of the pipe.

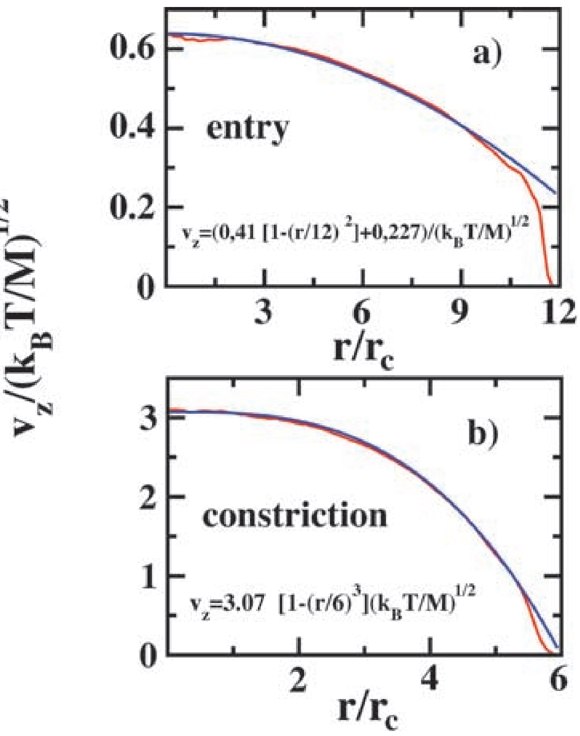

FIGURE 4 Velocity profiles in the presence of the constriction with periodic flow conditions. Panel (a) shows the profile prior to the constriction showing a good fit to a parabolic profile except close to the pipe boundary. Panel (b) depicts the profile within the constriction, better fit by a cubic dependence, demonstrating a spatial transient.

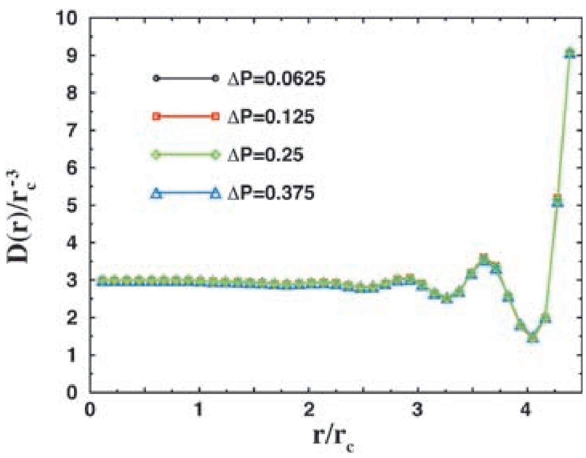

FIGURE 3 Mesoscopic particle density for a straight pipe configuration in the vicinity of the pipe wall. Density profiles correspond to monophasic fluid of $N = 3817$ particles, and $\rho = 3.0\,\mathrm{m}/r_c^3$. In these profiles we note an ordered structure close to the wall, due to the discreteness of the continuous phase. This effect occurs for radius r between 3.5 and 4.5 r_c. For values $r < 3.5\,r_c$ the values of the density profiles converges to the bulk value.

Once the correct monophase properties were verified we ran the full model including dispersed particles and constriction. The introduction of suspended particles in the analysis of the flow through a regular pipe, requires that their velocity profile, at low concentration of dispersed particles, match the velocity profile of the continuum phase. Otherwise, slipping between phases would ensue. Figure 5 depicts the profiles for a straight pipe geometry, for each kind of particles, determined for several values of ΔP and concentrations of the disperse phase. The two profiles match except for a region of the order of the dispersed particle diameter. This occurs in spite of the fact that no-slip is not guaranteed at the dispersed particle boundaries. Figure 5 shows a dispersed phase concentration of 5%. A slight increase in the concentration of the dispersion was found within the constriction indicating a tendency for the large particles to lag the continuous phase. Further exploration of this flow geometry is in progress, regarding concentration effects and eventual clogging of the constriction.

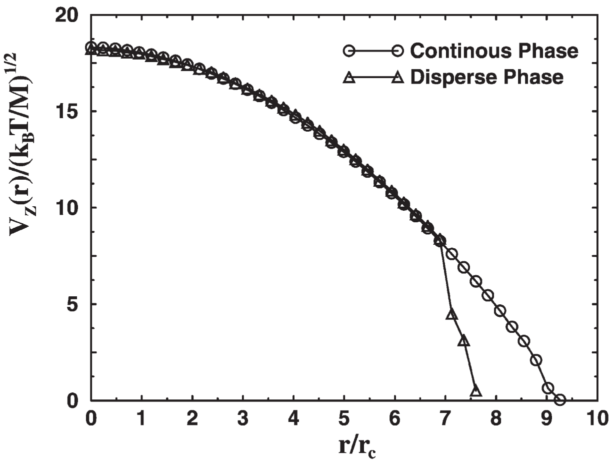

FIGURE 5 Suspended and continuous phase profiles in periodic flow conditions. The profiles correspond to dispersion at 5% of dispersed phase in a pipe of length $L = 60\,r_c$ and radius $R = 9.5\,r_c$. The mass density of the continuous phase is $\rho_{cp} = 3.0\,m/r_c^3$, the number of particles of the dispersed phase is $N_d = 25$, and the number of particles of the continuous phase is $N_{cp} = 49000$ particles. Note that the dispersed phase is dragged along by, the continuous phase suggesting non-slip conditions. The profiles are parabolic except for the values of r where discreteness of the dispersion becomes relevant.

SUMMARY AND CONCLUSIONS

We have used DPD method to emulate an incompressible suspension in a confined configuration. We propose a model to simulate a non-colloidal dispersion flowing in a constrained cylindrical geometry. Our model assumes that particles belonging to the continuum phase behave as pure DPD units while those from the disperse phase interact as conservative neutrally buoyant particles. The dispersed particles interact with the fluid through scaled DPD interactions.

Boundary conditions with cylindrical walls were included using "bounce back" reflections, which guaranteed no-slip at the boundary. In these conditions the model met with the expected behavior of an ideal Newtonian fluid for a regular cylindrical (constant radius) geometry. We found that modeling a boundary, within DPD, it is less advantageous to use frozen particles interacting via regular DPD forces since an artificial excluded volume arises, and the temperature of the system deviates from that fixed by the fluctuation dissipation theorem by as much a 20%.

When the motion of suspension were considered, non-slip conditions where not guaranteed between the continuous phase and the dispersed particles. Nevertheless, in practice the dispersed phase closely matched the continuous phase profile except close to the cylinder wall. As no rotations were considered this is sufficient condition to ensure non-slip.

In order to simulate a constriction we implemented a gradual decrease of the cylindrical radius forming a bottleneck. Longitudinal periodic boundary conditions were considered. The return of the dispersion to the Poiseuille profile after passing through the constrictions was achieved by prolonging the after-section of the cylinder conveniently. We showed that within the constriction, transient flow effects prevent the formation of a parabolic profile, which is substituted by a cubic profile closely resembling plug flow near the center.

These results allow us to conclude that the DPD model can successfully describe an isothermal, incompressible fluid in a cylindrical geometry under a pressure gradient and at constant flow conditions. This can be achieved provided appropriate non-slip boundary conditions are implemented as described above. In order to further approach real suspensions within our model, appropriate conservative forces between suspended particles should be included to describe both colloidal and non-colloidal systems. Such an improvement of the model will provide insight regarding the changes in a dispersion due to the presence of constrictions, of much interest in flow in porous media.

Acknowledgements

We acknowledge useful discussion with Vladimir Alvarado. This work was funded by the PDVSA-Intevep Emulsions project and by FONACII through grant S1-2001000910.

References

[1] Hoogerbrugge, P.J. and Koelman, J.M.V.A. (1992) "Simulating microscopic hydrodynamic phenomena whit disipative particle dynamics", *Europhys. Lett.* **19**, 155.
[2] Koelman, J.M.V.A. and Hoogerbrugge, P.J. (1993) "Dynamic simulations of hard-sphere suspensions under steady shear", *Europhys. Lett.* **21**, 363.
[3] Español, P. and Warren, P. (1995) "Statistical mechanics of dissipative particle dynamics", *Europhys. Lett.* **30**, 191.
[4] Coveney, P. and Novik, K.E. (1996) "Computer simulations of domain growth and phase separation in two-dimensional binary inmiscible fluids using dissipative particle dynamics", *Phys. Rev. E* **54**(5), 5134.
[5] Groot, R.D. and Warren, P.B. (1997) "Dissipative particle dynamics: bridgin the gap between atomistic and mesoscopic simulation", *J. Chem. Phys.* **107**(11), 4423.
[6] Español, P. (1997) "Fluid particle dynamics: a synthesis of dissipative particle dynamics and smoothed particle dynamics", *Europhys. Lett.* **39**, 605.
[7] Español, P. (1998) "A fluid particle model", *Phys. Rev. E* **57**(3), 2930.
[8] Español, P. (1995) "Hydrodynamics from dissipative particle dynamics", *Phys. Rev. E* **52**(2), 1734.
[9] Lees, A.W. and Edwards, S.F. (1972) "The computer study of transport processes under extreme conditions", *J. Phys. C: Solid State Phys.* **5**, 1921.
[10] Boek, E.S., Coveney, P.V. and Lekkerkerker, H.N.W. (1996) "Computer simulation of rheological phenomena in dense colloidal suspensions using dissipative particle dynamics", *J. Phys.: Condens. Matter* **8**, 9509.

[11] Boek, E.S., Coveney, P.V., Lekkerkerker, H.N.W. and van der Schoot, P. (1996) "Simulating the rheology of dense colloidal suspensions using dissipative particle dynamics", *Phys. Rev. E* **55**(3), 3124.
[12] Revenga, M., Zúñiga, I. and Español, P. (1999) "Boundary conditions in dissipative particle dynamics", *Comp. Phys. Commun.* **121**, 309.
[13] Revenga, M., Zúñiga, I., Español, P. and Pagonabarraga, I. (1998) "Boundary models in DPD", *Int. J. Mod. Phys. C* **9**(8), 1319.
[14] Marsh, C., "Theoretical aspects of dissipative particle dynamics" PhD Thesis, University of Oxford (Oxford).
[15] Marsh, C.A., Backx, G. and Ernst, M.H. (1997) "Fokker–Planck–Boltzmann equation for dissipative particle dynamics", *Europhys. Lett.* **38**, 411.
[16] Gardiner, C.W. (1985) *Handbook of Stochastic Processes for Physics, Chemistry and the Natural Sciences* (Springer Verlag, Berlin).
[17] McQuarrie, D. (1978) *Statistical Mechanics* (Harper Row, New York).
[18] Colmenares, P.J., unpublished.
[19] Allen, M.P. and Tildesley, D.J. (1987) *Computer Simulation of Liquids* (Clarendon Press, Oxford).