Magnetic drive micro / nanomotor model

S I Martynov¹ and L Y Tkach¹
¹Surgut State University, Polytechnical Institute, Surgut, Russia
E-mail: martynovsi@mail.ru

Abstract. A model of a micro- / nanomotor with a hydrodynamic mechanism of motion due to the action of a rotating uniform external magnetic field is proposed. Micro- / nanomotor - is a chain of three charged particles, one of which has a magnetic moment. The total charge of the system is zero. In the absence of an external field, the particles are in equilibrium due to the action of the forces of attraction and repulsion, which corresponds to the minimum interaction energy. After applying a rotating magnetic field, a particle with a magnetic moment begins to rotate, forming a flow in the surrounding viscous fluid. The flow induces a hydrodynamic force that moves the chain in a specific direction. The forces of hydrodynamic interaction of particles with each other are taken into account, as well as internal forces holding the particles together. The dynamics of six model aggregates with one rotating particle is simulated numerically. The proposed mechanism for moving the chain can be used in the design of micro- / nanomotors and control them to deliver the payload.

1. Introduction
Modern technologies are based on using the latest advances in the management of physical processes on a micro and nanoscale. Modern scientific advances in molecular biology and nanotechnology provide the potential for engineering development of nanomechanical systems with different functional capabilities at the present time. Biological and synthetic nanomotors are being actively studied [1, 2], which are planned to be used as guided vehicles for delivering cargo (therapeutic load, elements of self-assembled micro devices to their destination, etc.) both in natural and in laboratory conditions. Experiments are being conducted on the use of self-moving microparticles in medicine [3, 4] to isolate cancer cells. A large number of self-moving particles have the ability to self-organize [5], which allows you to control the formation of certain structures from them. Various synthetic nanomotors are created in the form of Janus-like particles [6, 7] that move due to chemical reactions [8, 9] in liquids that are fuel for such engines. Chemical reactions simultaneously supply fuel to the nanomotor and remove the products that they produce. Specially designed nanosized particles have the ability to move in external variables fields - electric [10], magnetic [11], ultrasonic [12, 13], chemical [14], photonic [15]. In all cases, the movement of the nanomotor occurs in a viscous fluid, which requires a more complete understanding of the hydrodynamic processes responsible for the formation of the required flow, which moves the nanomotor in a given direction.

The hydrodynamic mechanism of movement of aggregates of charged and dipole particles was proposed in the works [16, 17].

One of the characteristic structures that form in a fluid-particle system is a chain composed of particles interacting with each other. The formation of a chain is determined by the forces
of interaction acting directly between the particles. Therefore, it is of interest to consider the possibility of a controlled movement of a chain of particles in a viscous fluid as a result of the action of an alternating external field and to determine the parameters of the action that contribute to a more rapid movement of the chain in a viscous fluid. Such a study is also associated with the possible self-organization of particle chains into a new structure as a result of external influences and the determination of the parameters of influence to control such a process.

2. General assumptions and basic equations
Consider an aggregate consisting of three particles: a central particle B and two A, C located around the central particle B at a distance of 5.5a, where a is the characteristic scale Fig.1. The radii of the particles A, B and C are, respectively, k1a, k2a, k3a, where ki, i = 1, 2, 3 are the scale factors of the particle size.

The positive charge of particle B is equal to 2q, where q is the negative charge of each of the other two particles. The total charge of all three particles is zero, but the forces of the coulomb act between the particles. As mentioned above, for a stable equilibrium of the position of the center of particles, in addition to the Coulomb interaction, it is necessary to introduce an interaction not related to the charge of the particles. In this case, the interaction energy of particles in the aggregate is the sum of the energy of attraction between the central positively charged particle and each of the two negatively charged particles, the repulsive energy between the negatively charged particles and the repulsion energy of a non-electrical nature (see [16]). The total energy, for example, at the point occupied by particle A, has the form

\[ U = U_1 + U_2 + U_3, \quad U_1 = -k \frac{2q^2}{r_{BA}}, \quad U_2 = k \frac{q^2}{r_{CA}}, \quad U_3 = \frac{\gamma}{r_{BA}^3}. \]  

Here, \( k \) is the proportionality constant in Coulomb’s law and \( \gamma \) is the unknown coefficient determined by the condition that the forces in stable equilibrium are zero, \( U_1, U_2 \) are the potential energies of the Coulomb interaction of particle A with particle B and C, respectively, \( U_3 \) is potential energy of repulsion of non-Coulomb interaction of particle A with particle B. For the \( r_{BA} = r, r_{CA} = 2r \) the force acting of the particle A equals

\[ F_A = k \frac{2q^2}{r^2} - k \frac{q^2}{4r^2} - \frac{2\gamma}{r^3}. \]  

Since the considered position of the particles corresponds to equilibrium, the force must be equal to zero and we obtain

\[ \gamma = kq^20.48125a. \]  

It is possible to consider other cases when the charge of each particle has a different value and sign, but the aggregate as a whole must be charged neutrally, and the center of each particle is in a position of stable equilibrium.

We assume that particle A or C has a magnetic moment \( \mathbf{m} \). In a rotating uniform magnetic field, a particle also begins to rotate at a certain angular velocity \( \omega \), since its magnetic moment tends to orient itself along the applied field. The rotation of the particle causes the movement of the surrounding fluid, which leads to a violation of the equilibrium position of the particles. If the magnetic field is turned off, the system will return to its initial state of equilibrium within a characteristic relaxation time. But if not the magnetic field is turned off, but changes the direction of its rotation, then this leads to a change in the direction of rotation of a particle with a magnetic moment. In this case, the flow of the surrounding fluid initially promotes the return of the particles to the equilibrium position, but then removes them from this position in
a different direction than during the initial rotation. A change in the direction of rotation of the magnetic field with a certain period of time leads to periodic deformation of the chain. As a result, a flow is formed in the surrounding fluid, which creates a hydrodynamic force that moves the entire chain in a certain direction.

Spherical particles placed in an incompressible fluid of density \( \rho \) and viscosity \( \eta \). Particles can be of arbitrary radius and different density. It is assumed that interaction forces (attraction and repulsion) act between the particles, retaining them in an equilibrium position, in which the potential interaction energy \( U \) is minimal. We will consider the energy of particle interaction in the aggregate \( U \) as the sum of the energies of pairwise interactions of particles.

Since the dynamics of particles in a viscous fluid is considered and it is assumed that the particle sizes are small enough to consider the Reynolds number much less than unity and use the quasi-static approximation, then the equations for the dynamics of the fluid-particle system are written in the form [16]

\[
\nabla \mathbf{u} = 0, \quad -\nabla p + \eta \Delta \mathbf{u} = 0, \quad (4)
\]

\[
\mathbf{F}^{(i)}_k + \mathbf{F}^{(e)}_k + \mathbf{F}^{(h)}_k = 0, \quad \mathbf{T}^{(i)}_k + \mathbf{T}^{(e)}_k + \mathbf{T}^{(h)}_k = 0. \quad (5)
\]

Here, velocity \( \mathbf{u} \) and pressure \( p \) in a fluid, \( \mathbf{F}^{(h)}_k \) and \( \mathbf{T}^{(h)}_k \) are the forces and torques exerted on the particles by the fluid, \( \mathbf{F}^{(e)}_k \) and \( \mathbf{T}^{(e)}_k \) are the external forces and torques, and \( \mathbf{F}^{(i)}_k \) and \( \mathbf{T}^{(i)}_k \) are the internal forces and torques experienced by the \( k \)-th particle. Note that \( \mathbf{F}^{(i)}_k = -\nabla U_k \), where \( U_k \) is the energy of interaction of the particle with number \( k \) with all others. It is believed that the internal forces depend only on the relative position of the particles in the aggregate.

On the surface of particles with number \( k \), the adhesion conditions must be satisfied:

\[
u_i = V^k_i + \Omega^{k}_{ij} x^k_j, \quad |X^k| = a^k.
\] (6)

Here, the vector \( V^k \) denotes the absolute linear velocity, \( \Omega^{k}_{ij} \) is the angular velocity tensor, \( X^k \) is the position of an arbitrary liquid point relative to the center of the particle with number \( k \) and radius \( a^k \).

Away from the particle occurs perturbation attenuation

\[
u_i \rightarrow 0, \quad p \rightarrow p_0 \quad \text{if} \quad |X| \rightarrow \infty, \quad (7)
\]

where \( p_0 \) is the unperturbed pressure in the fluid.

To take into account the hydrodynamic interaction of particles in a fluid, the method proposed in [18] was used to determine the forces \( \mathbf{F}^{(h)}_k \) and \( \mathbf{T}^{(h)}_k \) torques. The method is based on representing the solution of fluid equations in the form of a multipole expansion with tensor coefficients and allows one to take into account the hydrodynamic interaction of a large number of particles in a viscous fluid. This approach is in good agreement with the experimental results [19].

To obtain the correct calculation results, we took into account the terms of the expansion with tensor coefficients of the sixth order. In computer simulation, the size of the particles, the viscosity of the carrier fluid, the magnitude of the external force acting on each particle, and its direction, as well as the time interval are set. Details of such a representation in modeling and the relationship between real and model parameters are presented in [16, 19].

3. Simulation results
Numerical simulation of the dynamics of six model chains of the structure considered above, in which one particle \( A \) has a magnetic moment \( \mathbf{m} \), is carried out. Models differ in particle size \( A \) and \( C \), particle size \( B \) is the same. A uniform magnetic field of strength \( \mathbf{H} \) is applied to the
system. Vector $\mathbf{H} = (0; -H \cos(\Omega t); -H \sin(\Omega t))$ rotates in the plane with frequency $\Omega$. The torque $\mathbf{m} \times \mathbf{H}$ acting on particle A is assumed to be the same for all six unit models.

As mentioned above, in the calculations, instead of real parameters of the problem, model ones are used. Therefore, the similarity method and model parameters were used. In computer simulation, the particle size $\hat{\mathbf{a}}$, viscosity of the carrier fluid $\hat{\eta}$, the value of the external moment $\hat{\mathbf{M}}$ acting on the particle with the magnetic moment $\hat{\mathbf{m}}$ and also the time interval $\hat{\mathbf{t}}$ are set.

The model and real density of the fluid are equal $\hat{\rho} = \rho = 1 \text{ g/cm}^3$. The model scale is $\hat{\mathbf{a}} = 0.1 \text{ cm}$, and the model viscosity of the fluid is $\hat{\eta} = 1 \text{ g/(cm} \cdot \text{s)}$. The particle sizes of the aggregates are shown in Table 1.

| Table 1. Particle sizes of aggregates. |
|---------------------------------------|
| Particle A | Particle B | Particle C |
| $1.5\hat{\mathbf{a}}$ | $2.5\hat{\mathbf{a}}$ | $3\hat{\mathbf{a}}$ |
| $1\hat{\mathbf{a}}$ | $2.5\hat{\mathbf{a}}$ | $2.5\hat{\mathbf{a}}$ |
| $1.5\hat{\mathbf{a}}$ | $2.5\hat{\mathbf{a}}$ | $1\hat{\mathbf{a}}$ |
| $2\hat{\mathbf{a}}$ | $2.5\hat{\mathbf{a}}$ | $1\hat{\mathbf{a}}$ |
| $2.5\hat{\mathbf{a}}$ | $2.5\hat{\mathbf{a}}$ | $1\hat{\mathbf{a}}$ |

Torque applied to particle A for all units is $\hat{M}=1.5 \text{ g} \cdot \text{cm}^2/\text{s}^2$. In order for the value of the torque $\hat{M}$ to be constant, it is necessary that the angle between the vectors $\hat{\mathbf{m}}$ and $\hat{\mathbf{H}}$ does not change. Since the magnetic moment is "frozen" into the particle, it is possible when particles A and vector $\hat{\mathbf{H}}$ rotate at the same angular velocities $\hat{\omega} = \Omega$. The equations of rotation of the model and real particles are written as follows

$$8K\pi \eta a^3 \omega = M, \quad 8K\pi \hat{\eta} \hat{a}^3 \hat{\omega} = \hat{M}. \quad (8)$$

Here, the coefficient $K$ characterizes the geometry of the structure and does not depend on the size of the particles in the structure. Since the magnetic moment of the particle is $m = M_s 4\pi a^3 / 3$, where $M_s$ is the saturation magnetization of the material of which the particle consists. Substituting the expression for the magnetic moment in these equations, we obtain

$$8K\pi \eta a^3 \omega = \frac{4\pi a^3}{3} M_s H, \quad 8K\pi \hat{\eta} \hat{a}^3 \hat{\omega} = \frac{4\pi \hat{a}^3}{3} M_s \hat{H}. \quad (9)$$

These equations give the relations between the real and the model parameters in rotation of particle

$$\frac{\eta \omega}{\hat{\eta} \hat{\omega}} = \frac{H}{\hat{H}}. \quad (10)$$

Another relation follows from the similarity of the flow during the rotational motion of particles

$$\frac{\rho \omega a^2}{\eta} = \frac{\hat{\rho} \hat{\omega} \hat{a}^2}{\hat{\eta}}. \quad (11)$$

The last two relationships give a relationship between the model and the real value of the magnetic field.
\[ H = \frac{\eta^2 \hat{a}^2}{\eta^2 \hat{a}^2} \dot{H}. \] (12)

We will assume that the rotating particle is made of a ferromagnetic material whose saturation magnetization \( M_s \) is 450 G. Knowing the size of the rotating particle \( \hat{a} \), we determine its magnetic moment \( \hat{m} \). Since the value of the torque \( \dot{M} \) is given, then from the equality \( \dot{M} = \hat{m} \dot{H} \) we obtain the model value of the magnetic field strength \( \dot{H} \). A change in the size of a rotating particle changes the magnitude of its magnetic moment and the model value of the applied magnetic field strength, since the torque is the same for all considered chain models. For a particle size \( \hat{a} = 0.1 \text{ cm} \) it follows that the model value of the magnetic field strength is \( \dot{H} = 0.796 \text{ Oe} \).

Let us take the value of the model particle charge such that \( kq^2 = \frac{20}{7} \cdot 10^{-13} \text{ N} \cdot \text{m}^2 \). This makes it possible to determine the model values of the forces of interaction between particles. Thus, the indicated parameters of the model make it possible to numerically simulate the dynamics of the considered six model chains with different particle sizes. The simulation was carried out using a special software package that poses and solves a system of equations and provides the result in a processed form.

In the absence of a magnetic field, the particles are in equilibrium on one straight line. It is believed that at the initial moment of time, the magnetic moment \( \hat{m} \) of particle \( A \) is also directed along the line. The rotating magnetic field is turned on perpendicular to line for 15 seconds. After that, the direction of rotation of the magnetic field is reversed and lasts 30 seconds. At the end of this time interval, the rotation of the magnetic field is reversed again and occurs within 30 seconds. After that, the specified cycle is repeated again. As mentioned above, such a cyclic action of the magnetic field leads to a cyclic deformation of the chain, similar to the movement of some swimming organisms, for example, tadpoles. The flow of the surrounding fluid caused by this deformation has a vortex character and leads to the appearance of a hydrodynamic force moving the chain along the line.

The numerical results obtained for the dynamics of the aggregates over a model time interval \( \hat{T} = 30 \text{ s} \) are given in Table 2. The table shows the calculated values of the parameters obtained for chains with particle sizes given in the corresponding rows of Table 1. The parameter \( \varepsilon \) indicates the computational error. Particle \( B \) movement indicated \( \Delta \hat{l} \). Inspection of Table 2 shows that the results depend substantially on the relative sizes of the particles.

| \( \hat{\omega}, s^{-1} \) | \( \Delta \hat{l}, \text{cm} \) | \( \varepsilon, 10^{-4} \) |
|----------------|----------------|----------------|
| 59.5897 | -0.01037 | 7.8415 |
| 59.4719 | -0.0200737 | 1.6064 |
| 59.4741 | -0.0111532 | 1.3225 |
| 17.4758 | -0.0113553 | 1.2619 |
| 7.24737 | -0.0117475 | 1.0064 |
| 3.58787 | -0.0126628 | 3.8657 |

The displacements of particles \( A \) and \( C \), located at the edges of the central particle \( B \), differ slightly in magnitude from the displacement of particle \( B \) due to the deformation of the aggregate as a result of the action of the hydrodynamic drag force during its motion in the liquid.

As can be seen from Tab. 2 the second unit moves faster than the others. Since the sum of the external forces exerted on the aggregate particles by the magnetic field is zero and the
internal forces cannot change the position of the center of gravity of the particle system, the motion of the aggregates is caused by the action of the hydrodynamic forces. The interaction of the particles leads to a flow in the surrounding viscous fluid, which creates a force moving the aggregate.

The values of the actual parameters can be determined using the updating formulas given in [16, 19]. For an aggregate of particles of size $a = 10^{-4}$ cm and for a fluid of actual viscosity $\eta = 10^{-2}$ g/(cm·s), we obtain $T = 3 \cdot 10^{-5}$ s. Taking into account the chosen model charge $kq = 20/7 \cdot 10^{-13}$ N and $k \approx 9 \cdot 10^3$ N·m²/C² yields the actual charge of the particles given by $q = 5.63 \cdot 10^{-17}$ C. From relations (11) and (12) we obtain real values of the angular velocity and magnetic field strength: $\omega = 10^4 \hat{\omega}$, $H = 100 \hat{H}$ Oe. Substituting the model value of the particle rotation speed from Tab. 2 we get the actual particle rotation speed. For the model value of the magnetic field $\hat{H} = 0.796$ Oe, we get that its real value is $H = 79.6$ Oe. The values of the real angular velocity and magnetic field strength can be reduced by decreasing the applied moment and increasing the time of exposure to the system.

4. Conclusion
The hydrodynamic mechanism of motion of a chain of three particles in a rotating magnetic field is considered. The particles of the chain are charged so that their total electric charge is zero, but at the same time they form a stable structure due to the Coulomb interaction of the particle charges and interaction of a non-electrical nature. One of the particles located relative to the central one has a magnetic moment. The rotating magnetic field causes this particle to rotate, creating a flow in the surrounding viscous fluid. This flow forms a hydrodynamic force, the action of which moves the chain in a certain direction. By changing the direction of rotation of the magnetic field, it is possible to control the motion of such a chain of particles. The hydrodynamic interaction of all particles in the chain is taken into account. Computer simulation of the movements of such aggregates in a viscous fluid was carried out using a specially developed software package. The numerical results from the simulations determine the frequency and magnitude of the applied magnetic field that causes the circuit to move. The proposed mechanism for moving a chain link can be used to create and control synthetic micro- or nanomotors.

Acknowledgments
The research was supported by grant of Russian Foundation for Basic Research No 18-41-860002/18.

References
[1] Montemagno C, Bachand G, Stelick S and Bachand M 1999 Nanotechnology 10 225
[2] Gao W and Wang J 2014 Nanoscale 6 10486
[3] Gao W, de Avila B E-F, Zhang L and Wang J 2018 Adv. Drug Deliv. Rev. 125 94
[4] Medina-Sanchez M, Xu H and Schmidt O G 2018 Therapeutic delivery. 9 4 303
[5] Lin Z, Gao C, Chen M, Lin X and He Q 2018 Current Opinion in Colloid Interface Science 35 51
[6] Paxton W F, Sen A and Mallouk T E 2005 Chemistry 11 22 6462
[7] Moran J L and Posner J D 2011 J. Fluid Mech. 680 31
[8] Nourhani A, Lammert P E, Crespi V H and Borhan A 2015 Phys. Fluid 27 012001
[9] FournierBidoz S, Arsenault A C, Manners I and Ozin G A 2005 Chem. Commun. 441
[10] Vissers T, van Blaaderen A and Imhof A 2011 Phys. Rev. Lett. 106 22 228303
[11] Dreyfus R, Baudry J, Roper M L, Fermigier M, Stone H A and Bibette J 2005 Nature 437 862
[12] Wang W, Castro L A, Hoyos M and Mallouk T E 2012 ACS Nano 6 6122
[13] Ahmed H, Destgeer G, Park J, Jung J H and Sung H J 2018 Adv. Sci. 5 1700285
[14] Robertsona B and Kapral R 2015 J. Chem. Phys. 142 15 10.1063
[15] He W, Frueh J, Hu N, Liu L, Gai M and He Q 2016 Adv. Sci. 3 1600206
[16] Martynov S I and Tkach L Yu 2019 Comput. Math. Math. Phys. 59 3 475
[17] Martynov S I and Tkach L Yu 2020 Comput. Math. Math. Phys. 60 11 1975
[18] Martynov S I 1998 Fluid Dyn. 33 245
[19] Martynov S I and Tkach L Yu 2015 Comput. Math. Math. Phys. 55 2 282