Supplementary Material (ESI) for Lab on a Chip

Magnetic Core Shell Nanoparticles Trapping in a Microdevice Generating High Magnetic Gradient

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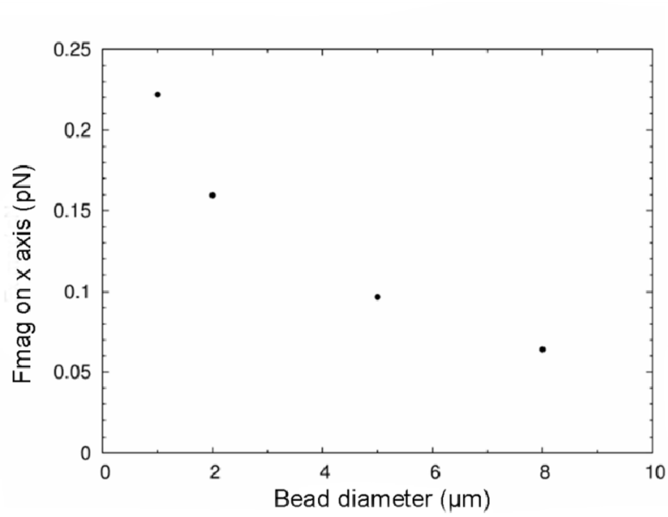

Figure S1**:** Evolution of $\boldsymbol{F_{mag}}$ on the x-axis in the magnetic chamber according to the iron beads diameter according numerical simulations using two square magnets (100 µm) in attraction with remnant ***B*** of 1T in the magnet.

SI 1: Finite element formulation of the magnetic field

The integral formulation is based on the local form given by Eq (1) from the paper using the scalar potential ϕ:

$$div\boldsymbol{B} = \nabla \bullet \left(-\mu\nabla\phi + \boldsymbol{B_0}\right) = 0 \qquad \text{(S1)}$$

Equation (S1) is derived in the global form (S2), using the Galerkin formulation frequently used in the finite element method (multiplication by a projective function α and integration on the domain of study).

$$\iint \left[\alpha\nabla \bullet \left(-\mu\nabla\phi + \boldsymbol{B_0}\right)\right] d\omega = 0 \qquad \text{(S2)}$$

By decomposing the product between α and the divergence in (S2), the second order derivative of the unknown ϕ (divergence of $\nabla\phi$) becomes:

$$\alpha\,\nabla \bullet (-\mu\nabla\phi + \boldsymbol{B_0}) = \nabla \bullet \left[\alpha\left(-\mu\nabla\phi + \boldsymbol{B_0}\right)\right] - \nabla\alpha \bullet \left(-\mu\nabla\phi + \boldsymbol{B_0}\right) \qquad \text{(S3)}$$

Equation (S3) is applied in (S2) and the Ostrogradsky theorem is used to reject the divergence term $\nabla \bullet \left[\alpha\left(-\mu\nabla\phi + \boldsymbol{B_0}\right)\right]$ at the boundary in (S4) where it equals to zero (no magnetic field at the external boundaries of the domain due to the use of a large “air box”).

$$\iint \left[\nabla\alpha \bullet \left(\mu\nabla\phi - \boldsymbol{B_0}\right)\right] d\omega + \int \alpha\,\boldsymbol{B} \bullet n\; d\omega = 0 \qquad \text{(S4)}$$

The unknown vector ϕ is interpolated with a function β of the same type as the projective function α as the Galerkin method is used. It leads to the final form (S5) where the first term corresponds to the matrix to invert, the second term being the source term (discretization non described).

$$\iint \mu \nabla\alpha \bullet \nabla\beta \, \phi \, d\omega = \iint \nabla\alpha \bullet \boldsymbol{B_0} \, d\omega \qquad \text{(S5)}$$

SI 2: Numerical model and assumptions

Numerical simulations, based on the finite elements method (FEM), were carried out in 2D geometries with the commercial software Flux-Expert™ (Astek Rhône-Alpes) on a Mac Pro with Ubuntu Linux 7.10 operating system.

In the case of permanent magnets and in the absence of charges in movement, the magnetic field $\boldsymbol{H}$ is irrotational and as the calculation domain is simply connected, $\boldsymbol{H}$ derives from a scalar magnetic potential ϕ ($\boldsymbol{H} = -\nabla\phi$). As the magnetic flux density $\boldsymbol{B}$ is conservative, the equation to be solved using a Galerkin formulation (Supporting information, *SI 1*) is written as:

$$\mathrm{div}\,\boldsymbol{B} = \nabla \bullet (-\mu\nabla\phi + \boldsymbol{B_0}) = 0 \tag{4}$$

Where $\boldsymbol{B_0}$ represents the magnetic flux density imposed in the magnet and μ the permeability. The magnetic force acting on a magnetic dipole moment $\boldsymbol{m}$ can be expressed as the gradient of the magnetic potential energy U. If we assume $\boldsymbol{m}$ constant, this force is simply given by:

$$\boldsymbol{F_m} = -\nabla(U) = \nabla(\boldsymbol{m} \bullet \boldsymbol{B}) = (\nabla\boldsymbol{m}) \bullet \boldsymbol{B} + \boldsymbol{m} \bullet \nabla\boldsymbol{B} \approx (\boldsymbol{m} \bullet \nabla)\boldsymbol{B} \tag{5}$$

In the case of superparamagnetic nanoparticles in a non-magnetic medium like pure water, the magnetic dipole moment can be written as $\boldsymbol{m} = V\boldsymbol{M} = V\chi\boldsymbol{H}$. As $\boldsymbol{H}$ and $\boldsymbol{B}$ only differ by the constant μ_0, the magnetic force can finally be written as Eq.

The following assumptions are made: (a) magnetostatic conditions ($\partial\boldsymbol{B}/\partial t=0$ and no external source of electric or magnetic field), (b) homogeneous media (μ uniform in every domain), (c) air box big enough for not perturbing the magnetic field distribution, (d) constant magnetic susceptibility of the particles and magnetic moment assumed to be unsaturated, (e) static particle solution in the microchannel (no flow), (f) particles have no influence on the magnetic field and (g) interactions between particles are not considered.

SI 3: Numerical parameters

The magnetic flux density and force were calculated in a 2D geometry for a reference system. It is composed of a microchannel (30 µm high and 100 µm long) closed by insulating layers (35 µm high and 100 µm long), surrounded by two permanent square micromagnets (100 µm), providing a spacing of 100 µm between the two magnets. The whole reference system is placed in an air box, enabling the magnetic field to rotate freely from one pole to the other. The total proportions of the system are a length of 600 µm for a height of 800 µm. One (or more) column composed of 12 ferromagnetic beads spaced by 0.1 µm is placed vertically in the middle of the microchannel. The mesh size (δ) was chosen according to the criteria previously validated,[1] that is to say less than 1/20 of the channel height in the microchannel and less than 1/20 of the magnet length for the edges of the magnets. For the ferromagnetic beads, δ = 0.2 µm (1/10 of bead diameter).

The numerical parameters are:

$\mu_0 = 1.256 \times 10^{-6}$ [H/m]

$\boldsymbol{B_0}$ (perpendicular to the microchannel) = 1 [T]

Magnetic susceptibility of nanoparticles $\chi_{nano} = 0.01$ [-]

Magnetic susceptibility of iron beads $\chi_{ferro} = 3.9$ [-]

Magnetic susceptibility of polystyrene magnetic beads $\chi_{poly} = 1$ [-]

Nanoparticles diameter $d_{nano} = 30$ [nm]

Iron beads diameter $d_{ferro} = 2$ [μm]

Polystyrene magnetic beads diameter $d_{poly} = 2$ [μm]

References

1 A-L. Gassner, M. Abonnenc, H. X. Chen, J. Morandini, J. Josserand, J. S. Rossier, J-M. Busnel and H. H. Girault, *Lab Chip*, 2009, **9**, 2356–2363.