Albrecht Bertram
Jürgen Tomas
Editors

Micro-Macro-Interactions

in Structured Media and Particle Systems

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Jürgen Tomas

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In Structured Media and Particle Systems

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Preface

It is a common feature of many materials and media that their behaviour is much better understood on a micro level than on the macro level, on which engineers normally work for designing technical parts, machines, apparatuses, or engineering systems. In such cases it is advantageous to study and compare the behaviour on both scales, the micro and the macro scale. Such micro-macro transitions have become rather successful and customary during the last decade, perhaps stimulated by the increasing computational power nowadays available. We are now capable to model the micro behaviour in detail, and to accomplish the micro-macro transition or homogenisation numerically. One of the most successful methods in many technological branches is the Representative Volume Element technique (RVE), where only a small representative part on the micro scale is modelled and used for the determination of the macro values of the physical variables like, e.g., forces, strains, heat fluxes, solid or liquid phase distributions, etc.

In the present volume we have collected results of such micro-macro investigations from more than half a decade of joint research work in different branches of engineering, in particular on

- the inelastic material behaviour of polycrystals;
- fibre and particle reinforced composites;
- solids under thermal loads;
- particle contacts and dynamics of particle systems.

The distributions of this book have been collected in four parts, according to these four fields of application, although many of them combine methods from different approaches and, thus, belong to more than just one of the above topics.

In all contributions, the behaviour of micro structures determines the macro behaviour of the system or medium. This micro structure may consist of

- different grains or phases of solids in polycrystalline materials,
- assemblies of matrix material and reinforcement in composites,
- solid particles moving in fluids,
- mixtures of interacting particles or liquids and gases in porous solid media,

etc. However, despite of the large manifold of different media and fields, the reader will detect common methods, algorithms, and models, which have been applied in rather different areas. The range of the applications spans from microphysics, material science, to mechanical engineering and process engineering, including numerical and mathematical methods. Such results can only be expected, if experts from physics, mathematics, and engineering cooperate and exchange knowledge, methods, and models within one joint research project.

All the presented results stem from investigations which have been performed at the Graduate School within the Otto von Guericke University Magdeburg during the period of 2001 - 2008 supported by the German Science Foundation (DFG) and the Land Sachsen-Anhalt under grant GK 828.

Magdeburg, June 2008

A. Bertram
J. Tomas

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Numerical Study of the Influence of Diffusion of Magnetic Particles on Equilibrium Shapes of a Free Magnetic Fluid Surface

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Abstract. A general mathematical model and a computational method is proposed for studying the influence of the particle diffusion on equilibrium shapes of a magnetic liquid. It is applied on the ferrohydrostatic problem of equilibrium shapes of a magnetic liquid in a cylindrical cavity subject to a magnetic field created by a cylindrical permanent magnet located below the cavity. Numerical simulations show that the usual assumption of a uniform concentration field does not apply in the case of high-gradient magnetic fields.

1 Introduction

Because of their ability for ponderomotive interaction with an external magnetic field, magnetic fluids have not only provoked the development of a new direction in fluid mechanics but have become a new technological material which found a wide application in engineering [1, 3, 4, 9]. A magnetic fluid is a stable colloidal suspension of ferromagnetic particles in a carrier liquid (oil, water, bio-compatible liquid). The size of particles is of the order of 10^{-8}m, and they are in the Brownian motion state in the carrier liquid. In modelling magnetic fluids often a uniform distribution of particles has been assumed. However, owing to the fact that the particle possess magnetic properties, not only Brownian motion but also a magneto-phoresis diffusion process takes place in a magnetic fluid [5, 9]. This diffusion process becomes significant when the magnetic fluid is under the influence of a high-gradient magnetic field.

The main objective of this work is the investigation of the influence of diffusion of magnetic particles on equilibrium axisymmetric shapes of a free magnetic-fluid surface. As an example, we will consider the problem of equilibrium shapes of a magnetic fluid in a cylindrical cavity subject to a magnetic field created by a cylindrical permanent magnet located below the cavity. As the fluid magnetization value is directly proportional to the particle concentration in the fluid volume [2, 3, 7, 9], which is determined by the magnetic field structure, the diffusion effect is expected to become appreciable under a strongly non-uniform magnetic field.

2 Mathematical Model

Under the assumptions that the influence of the gravity force on the diffusion of Brownian particles is negligible and that the magnetic particles are of spherical form and of equal size, the magnetic particle mass transfer in a magnetic fluid can be described by the equation [2, 7]

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C = D\nabla \cdot \left(\nabla C - CL(\xi H)\nabla(\xi H)\right), \tag{1}$$

where C is the volume concentration of the particles in the colloid; t the time variable; $\mathbf{v}$ the velocity of a convective motion; D the diffusion coefficient; H the magnetic field intensity; $\xi = \frac{\mu_0 m_m}{kT}$, $\mu_0 = 4\pi \times 10^{-7} \mathrm{Hm}^{-1}$ is the magnetic constant (magnetic permeability of vacuum); m_m the magnetic moment of a particle; $k = 1.3806568 \times 10^{-23} \mathrm{JK}^{-1}$ the Boltzmann constant; T the particle temperature; m the mass of a particle; and

$$L(\xi H) = \coth \xi H - \frac{1}{\xi H}$$

the Langevin function. We assume that the fluid is incompressible and the boundary is impermeable, thus $\operatorname{div} \mathbf{v} = 0$ inside the fluid, $\mathbf{v} \cdot \mathbf{n} = 0$ on fixed walls, $\mathbf{v} \cdot \mathbf{n} = v_\Gamma$ on the free surface, where $\mathbf{n}$ denotes the outer unit normal at the boundary and v_Γ the velocity of the free surface. Equation (1) is supplemented with the condition of impermeability of boundaries by particles

$$\frac{\partial C}{\partial n} - C\xi L(\xi H)\frac{\partial H}{\partial n} = 0\,. \tag{2}$$

Moreover, a uniform concentration at the initial state,

$$C = C_0 = const\,, \quad t = 0 \tag{3}$$

is prescribed. Equation (1) together with condition (2) and (3) represent the mathematical model of the diffusion process of ferromagnetic particles in a magnetic fluid. Notice that the solution of the problem (1)-(3) satisfies the condition of conservation of the mean concentration:

$$\frac{1}{V}\int_V C\,dV = C_0 \quad \text{for all} \quad t \ge 0\,,$$

where V is the fluid volume (or the spatial domain of definition of the problem).

For $t \to \infty$ we obtain the steady-state concentration problem with $\mathbf{v} = \mathbf{0}$ which can be written in the form

$$\begin{gathered} \nabla\left(\nabla C - C\nabla(\ln\varphi)\right) = 0 \text{ inside the fluid,} \\ \frac{\partial C}{\partial n} - \frac{\partial(\ln\varphi)}{\partial n} = 0 \text{ at the boundary,} \\ \int_V C\,dV = VC_0\,, \text{ where } \varphi = \frac{\sinh \xi H}{\xi H} \end{gathered} \tag{4}$$

As show in [7], the problem (4) admits an analytical solution given by

$$C = \varphi \frac{C_0 V}{J_0}, \quad J_0 = \int_V \varphi dV . \tag{5}$$

The magnetic properties of the magnetic fluid are determined by its magnetization M which depends on both the magnetic field intensity H and the particle concentration C. In ferrohydrodynamics [2, 3, 7, 9], Langevin's magnetization law for a non-uniformly concentrated magnetic fluid is defined by the formula

$$M = M(H, C) = \frac{M_s}{C_0} L(\xi H) C \tag{6}$$

where M_s is the magnetic-fluid saturation magnetization; C_0 the mean concentration corresponding to a uniform distribution of the particles.

The equilibrium shapes of a free magnetic-fluid surface are described by the Young-Laplace equation. In the static case, it takes the form

$$\sigma_0 K = \frac{1}{2}\mu_0 \left(\frac{M}{H} H_n \right)^2 + \mu_0 \int_0^H M dH + p_f - p_0 \tag{7}$$

where K is the sum of principal free-surface curvatures which is positive if the surface is convex; σ_0 the surface tension coefficient, p_0 the pressure in a surrounding non-magnetic medium; p_f the thermodynamic pressure in the fluid.

Equation (7) is supplemented with boundary conditions as well as with the non- local (integral) condition of fluid volume conservation. As boundary conditions we have either conditions where the fluid contacts a solid wall specified by the wall geometry and a given wetting angle, or the symmetry condition at the rotation axis.

Let us now apply our model to a specific example. We consider a fixed volume of a magnetic fluid filling a cylindrical cavity. Let R_c be the radius of the cavity and

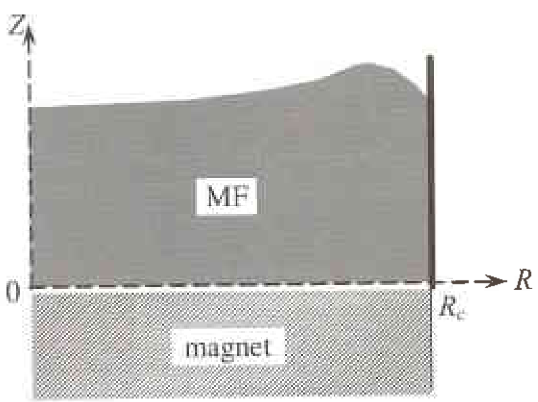

Fig. 1. Illustration of the problem

magnet, and let V denote the fluid volume. The free surface is supposed to by axisymmetric, its shape is completely determined by the equilibrium line. We introduce cylindrical coordinates R, Z and parametrise the equilibrium line with respect to the arc length S that takes the value S=0 at the symmetry axis Z=0 and $S=l$ at the solid wall $R= R_c$. Then, the equilibrium line is given by the parametric functions ($R(S)$, $Z(S)$). Note that the tangent vector $\tau = (R', Z')$ is oriented in the direction of increasing S. The surface curvature is defined by $K = -(RZ')'/(RR')$, where the prime stands for differentiation with respect to S. Natural boundary conditions corresponding to a contact angle of $\pi/2$ for (7) are the following

$$\begin{aligned} R(0) &= 0, \quad R'(0) = 1, \quad Z'(0) = 0, \\ R(l) &= R_C, \quad R'(l) = 1, \quad Z'(l) = 0. \end{aligned} \tag{8}$$

Note that also different values of the contact angle can be handled by our method. The given volume V is determined as the volume of a body of revolution and gives the constraint

$$V = 2\pi \int_0^l ZRR' dS . \tag{9}$$

The magnetic field is created by a permanent magnet having the form of a circular cylinder, see Fig1. In this case an analytical solution is known [8].

$$\begin{aligned} H_z &= \frac{M_c}{2\pi} \sum_{k=1}^{2} (-1)^k \int_{R-R_c}^{R+R_c} \frac{Z_k}{X^2 + Z_k^2} \sqrt{\frac{R_c^2 - (X-R)^2}{R_c^2 + Z_k^2 + 2XR - R^2}} dX, \\ H_r &= \frac{M_c}{2\pi} \sum_{k=1}^{2} (-1)^k \int_{R-R_c}^{R+R_c} \frac{X}{X^2 + Z_k^2} \sqrt{\frac{R_c^2 - (X-R)^2}{R_c^2 + Z_k^2 + 2XR - R^2}} dX, \end{aligned} \tag{10}$$

$$Z_1 = Z - h_C, \qquad Z_2 = Z - h_C .$$

Here, h_c denotes the half-height of the magnet and M_c is its magnetization. These formulas satisfy the Maxwell equation and describe the field in the whole space except in a narrow neighbourhood of the magnet. We will neglect the magnetization of the ferrofluid due to $M \ll H$, and apply these formulas in the domain filled with the ferrofluid.

Next we choose the arclength l of the equilibrium line as a characteristic dimension and introduce dimensionless variables

$$s = \frac{S}{l}, \quad z = \frac{Z}{l}, \quad r = \frac{R}{l}, \quad h = \frac{H}{M_c}, \quad \overline{C} = \frac{C}{C_0}.$$

Then, we can reformulate (7)-(9) in the dimensionless form

$$\begin{aligned} &z''=r'F, && r''=-z'F, && 0\le s\le 1,\\ &r(0)=0, && r'(0)=1, && z'(0)=0,\\ &r(1)=\left(\frac{I_0}{U}\right)^{1/3}, && r'(1)=1, && z'(1)=0. \end{aligned} \tag{11}$$

A new condition for z at $s = 1$ can be obtained by integrating (9) by parts $z(1)=\dfrac{1}{\pi r^2(1)}(I_0+I_1)$.

Finally, the dimensionless magnet field can be derived form (10) to be

$$\begin{aligned} h_z &= \frac{r^2(1)}{2\pi}\int_{-1}^{1}[\sqrt{1-t^2}(z^-\xi^- - z^+\xi^+)]\,dt,\\ h_r &= \frac{r^2(1)}{2\pi}\int_{-1}^{1}\left[\sqrt{1-t^2}(r(1)t+r)(\xi^- - \xi^+)\right]dt. \end{aligned} \tag{12}$$

Here the following abbreviations have been used

$$F=\left[-\phi(\overline{C},h,s)+\gamma\right]-\frac{z'}{r},\qquad \phi(\overline{C},h,s)=\frac{A_1}{r(1)}\overline{C}+\frac{1}{2r(1)}A_3\left(\overline{C}L(A_2h)\frac{h_n}{h}\right)^2,$$

$$\overline{C}=\varphi(A_2h)\frac{I_0}{J_0},\qquad J_0=\int_v \varphi dv,\qquad I_0=2\pi\int_0^1 zrr'ds,\qquad I_1=2\pi\int_0^1 z'\frac{r^2}{2}ds,$$

$$\xi^{\pm}=\frac{1}{\left[(r(1)t+r)^2+(z^{\pm})^2\right]\sqrt{r^2(1)+(z^{\pm})^2+r^2+2r(1)tr}},\qquad z^{\pm}=z\pm r(1)P,$$

$$A_1=\frac{\mu_0 M_s R_c}{\xi\sigma_0},\quad A_2=\xi M_c,\quad A_3=\frac{\mu_0 M_s^2 R_c}{\sigma_0},\quad U=\frac{V}{R_c^{\,3}},\quad P=\frac{h_c}{R_c}.$$

The solution $z(s)$, $r(s)$ of the dimensionless problem (11), (12) is determined by dimensionless parameters A_1, A_2, A_3, U, P and the undefined constant γ.

3 Computational Algorithm

Following the strategy in [6], we construct a difference scheme of second-order approximation on the uniform grid $\{s_i = ih \mid i = 0,1,\ldots,N;\ h=1/N\}$ for the problem (11)-(12). We will denote the solution of the difference scheme by the same letters as the corresponding solution of the differential equation

$$\begin{aligned}
&\Lambda_1(r,z,F)|_i = r_{\bar{s}s,i} + z_{\dot{s},i}F_i = 0, \quad i=2,\dots,N-1\\
&\Lambda_2(r,z,F)|_i = z_{\bar{s}s,i} - r_{\dot{s},i}F_i = 0; \quad i=1,\dots,N-1\\
&r_1 = h, \qquad r_{\bar{s},N} = 1;\\
&z_{\bar{s},0} = \frac{h}{2}F_0, \quad z_N = \frac{1}{\pi}\left(\frac{U}{I_0}\right)^{2/3}(I_0+I_1);
\end{aligned} \tag{13}$$

where

$$\begin{aligned}
&F_i = F(r_i, z_i, r_{\dot{s}}, z_{\dot{s}}), \quad i=1,\dots,N-1;\\
&F_0 = F(z_0), \quad i=0;\\
&r_{s,i} = (r_{i+1}-r_i)/h, \qquad r_{\bar{s},i} = (r_i - r_{i-1})/h,\\
&r_{\dot{s},i} = (r_{i+1}-r_{i-1})/(2h), \quad r_{\bar{s}s,i} = (r_s - r_{\bar{s}})/h.
\end{aligned}$$

The integrals I_0 and I_1 are evaluated by the trapezoidal rule. For the calculation of the magnetic field components (12) a Gaussian quadrature rule has been used. The non-linear difference problem (13) has been solved by the two-layer iteration scheme

$$\begin{aligned}
&\frac{1}{\tau}(r^{n+1}_{\bar{s}s,i} - r^{n}_{\bar{s}s,i}) + \Lambda_1(r^n, z^n, F^n)|_i = 0; \quad i=2,\dots,N-1;\\
&r_1^{n+1} = h, \quad r^{n+1}_{\bar{s},N} = 1;\\
&\frac{1}{\tau}(z^{n+1}_{\bar{s}s,i} - z^{n}_{\bar{s}s,i}) + \Lambda_2(r^n, z^n, F^n)|_i = 0; \quad i=1,\dots,N-1;\\
&z^{n+1}_{\bar{s},0} = \frac{h}{2}F_0^n, \quad z_N^{n+1} = \frac{1}{\pi}\left(\frac{U}{I_0^n}\right)^{2/3}(I_0^n + I_1^n);
\end{aligned} \tag{14}$$

Here, $n = 0,1,\dots$ is the iteration number; $\tau > 0$ is a relaxation parameter. The two-layer iteration scheme (14) is requires in each iteration step the solution of linear tridiagonal systems which has been done by means the three-point elimination method (Thomas algorithm).

4 Numerical Results

The numerical study has been performed for fixed values $A_1 = 8$, $A_3 = 6.5$, $P = 1$, the two values U=0.07 and U=2 corresponding two different fluid volumes, and for a wide range of the parameter A_2 characterizing the magnitude of the magnetization of the permanent magnet. In order to study the influence of the diffusion process, computation have been carried out by assuming both a uniform distribution of the particle in the fluid and taking the diffusion effect into consideration.

The diffusion effect of particles can clearly be seen in Fig. 2 which represents the axisymmetric equilibrium shapes for a small volume U=0.07 and A_2=4. The magnetic field strength along the free surface shape differs for different fluid volumes and influences its shape as can be seen by comparing Fig. 2 and Fig. 3. Moreover, in Fig. 3,

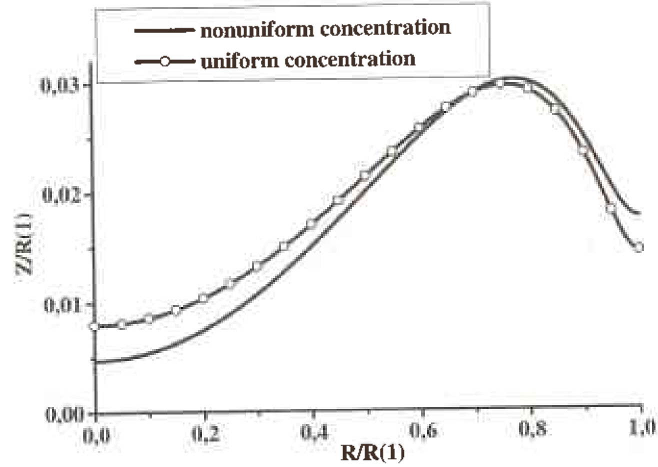

Fig. 2. Free surface shapes for $A_2 = 4$ and U=0.07

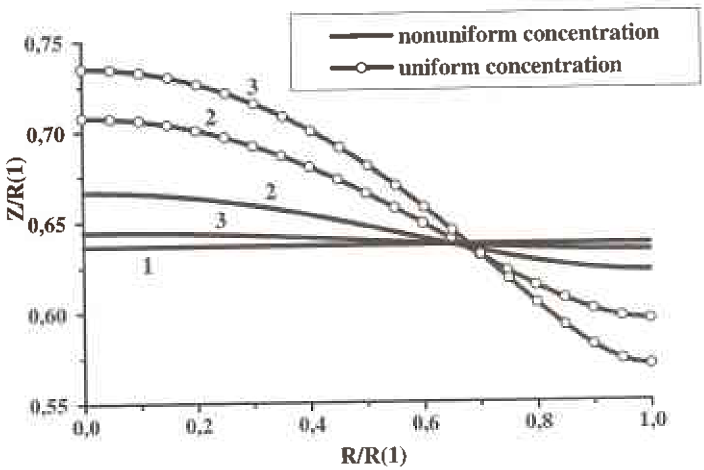

Fig. 3. Free surface shapes U=2: $1 - A_2 = 0$; $2 - A_2 = 2$; and $3 - A_2 = 4$

in which characteristic equilibrium shapes for three values of A_2 are shown, we detect a new property. For higher values of the parameter A_2 a distinction between the free surfaces with uniform and non-uniform particle concentration can be observed. Starting with small values of the parameter A_2 and increasing it, both curves move in the same direction. Then, the curve corresponding to a non-uniform particle concentration reaches a "critical" position, after which it starts to move in the opposite direction. As we can see in Fig. 4 the particle concentration far from the magnet becomes close to zero for increasing values of A_2 and does not influence considerably the free surface shape.

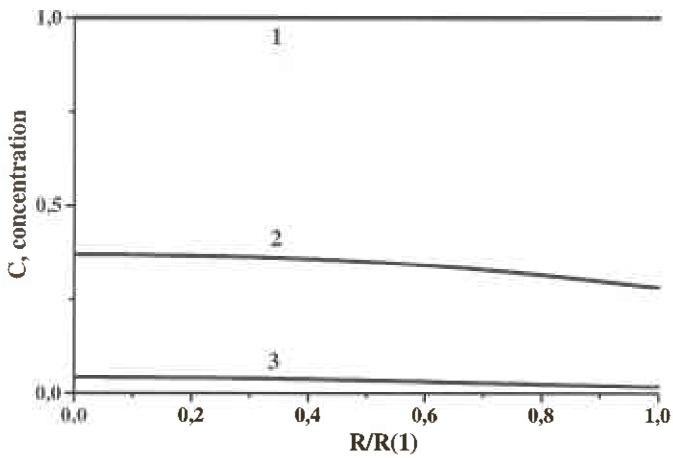

Fig. 4. Distribution of concentration at a free surface for U=2: 1 – $A_2 = 0$; 2 – $A_2 = 2$; and 3 – $A_2 = 4$

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Micro-Macro-Interactions
Albrecht Bertram, Jürgen Tomas (Eds.)

Many materials or media in nature and technology possess a microstructure which determines their macroscopic behaviour. The knowledge of the relevant mechanisms is often more comprehensive on the micro than on the macro scale. On the other hand, not all information on the micro level is relevant for the understanding of the macro behaviour. Therefore, averaging and homogenization methods are needed to select only the specific information from the micro scale, which influences the macro scale. These methods also open the possibility to design or to influence microstructures with the objective to optimize their macro behaviour.
This book presents the development of new methods in this interdisciplinary field of micro-macro-interactions of engineering as well as applied mathematics and physics. In particular, solids with microstructures and particle systems are considered.

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