THEORETICAL ASPECTS OF MICROCHANNEL ACOUSTOPHORESIS: THERMOVISCOUS CORRECTIONS TO THE RADIATION FORCE

Henrik Bruus
Department of Micro- and Nanotechnology, Technical University of Denmark, DTU Nanotech Buildig 345 B, DK-2800 Kongens Lyngby, Denmark

Summary The acoustic radiation force is calculated for the case of an ultrasound wave scattering on a compressible, spherical particle suspended in a viscous, thermal conducting fluid. Using Prandtl–Schlichting boundary-layer theory, we include the viscosity and the volume thermal expansion coefficient of the fluid and derive an analytical expression for the radiation force. The resulting force (valid for particle radius and boundary layers much smaller than the acoustic wavelength) is analyzed for microchannel acoustophoresis.

BACKGROUND AND GOVERNING EQUATIONS

With recent developments in microfabrication technologies allowing for integration of ultrasound resonators in lab-on-a-chip systems, the acoustic radiation force has received renewed attention as a label- and contact-free way to manipulate particles [1, 2]. Traditionally, the acoustic radiation force has been modeled using the inviscid theory of the acoustic radiation force. This approach is approximately correct for particles (radius a) much larger than the thicknesses δ and δ_{th} of the viscous and thermal boundary layers, in which dissipation plays a dominant role. However, with the recent experimental advances, studies of smaller particles, and improved accuracy, it is relevant to re-visit the theoretical analysis.

A general mathematical expression for the acoustic radiation force (wavelength λ) with thermoviscous corrections is given by Doinikov [3]. However, he presented analytical results in closed form only for particles with a thick boundary layer ($a \ll \delta, \delta_{\mathrm{th}} \ll \lambda$) and with a thin boundary layer ($\delta, \delta_{\mathrm{th}} \ll a \ll \lambda$). Here, we extend his analysis and present analytical results in closed form for any particle size ($a, \delta, \delta_{\mathrm{th}} \ll \lambda$). The resulting radiation force is analyzed using parameter values typically employed in microparticle acoustophoresis in microchannels. Briefly, and to establish our notation [4], the full acoustic problem in a fluid, which before the presence of any acoustic wave is quiescent with constant temperature T_0, density ρ_0 and pressure p_0, is described by the four scalar fields pressure p, temperature T, density ρ and entropy per mass unit s as well as the single velocity vector field $\boldsymbol{v}$. The two thermodynamic relations

$$\mathrm{d}\rho = \frac{\gamma}{c_0^2}\,\mathrm{d}p - \alpha\rho\,\mathrm{d}T, \quad \text{and} \quad \mathrm{d}s = \frac{c_p}{T}\,\mathrm{d}T - \frac{\alpha}{\rho}\,\mathrm{d}p, \quad \text{with} \quad \alpha = -\frac{1}{\rho_0}\left(\frac{\partial\rho}{\partial p}\right)_p, \tag{1}$$

can be used to eliminate ρ and s, so that we only need to deal with the acoustic perturbations in temperature T, pressure p, and velocity $\boldsymbol{v}$. Here c_0 is the (isentropic) sound speed, c_p the specific heat at constant pressure, and γ (= 1.01 for water at 293 K) is the ratio of specific heats . To first and second order (subscript 1 and 2, respectively) we have

$$T = T_0 + T_1 + T_2, \qquad p = p_0 + p_1 + p_2, \qquad \text{and} \qquad \boldsymbol{v} = \boldsymbol{v}_1 + \boldsymbol{v}_2. \tag{2}$$

To first order, the thermodynamic heat transfer equation for T_1, the kinematic continuity equation expressed in terms of p_1, and the dynamic Navier–Stokes equation for the velocity field $\boldsymbol{v}_1$, become

$$\partial_t T_1 = D_{\mathrm{th}}\nabla^2 T_1 + \frac{\alpha T_0}{\rho_0 c_p}\,\partial_t p_1, \quad \partial_t p_1 = \frac{\rho_0 c_0^2}{\gamma}\Big[\alpha\partial_t T_1 - \boldsymbol{\nabla}\cdot\boldsymbol{v}_1\Big], \quad \rho_0\partial_t\boldsymbol{v}_1 = -\boldsymbol{\nabla}p_1 + \eta\nabla^2\boldsymbol{v}_1 + \beta\eta\,\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v}_1). \tag{3}$$

Here (with values for water at room temperature given in parenthesis), D_{th} is the thermal diffusivity (1.43×10^{-7} m^2/s), α is the volume thermal expansion coefficient (2.07×10^{-4} K^{-1}, c_p is the heat capacity (4.18×10^3 J kg^{-1}K^{-1}), ρ_0 is the density (998 kg/m^3), η is the dynamic viscosity (10^{-3} Pa s), and β is the viscosity ratio ($\approx$ 1.7). A further simplification can be obtained when assuming all first-order fields to have harmonic time dependence $\mathrm{e}^{-\mathrm{i}\omega t}$, because then p_1 can be eliminated inserting Eq. (3b) with $\partial_t p_1 = -\mathrm{i}\omega p_1$ into Eq. (3a) and (c). After using the thermodynamic identity $T_0\alpha^2 c_0^2/c_p = \gamma - 1$, we arrive at

$$\mathrm{i}\omega T_1 + \gamma D_{\mathrm{th}}\nabla^2 T_1 = \frac{1-\gamma}{\alpha}\,\boldsymbol{\nabla}\cdot\boldsymbol{v}_1, \qquad \text{and} \qquad \mathrm{i}\omega\boldsymbol{v}_1 + \nu\nabla^2\boldsymbol{v}_1 + \nu\left[\beta + \mathrm{i}\frac{c_0^2}{\gamma\nu\omega}\right]\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v}_1) = \frac{c_0^2\alpha}{\gamma}\,\boldsymbol{\nabla}T_1. \tag{4}$$

From Eq. (4) arise the thermal and the viscous penetration depth δ_{th} and δ, respectively (values for 1 MHz in water),

$$\delta_{\mathrm{th}} = \sqrt{\frac{2D_{\mathrm{th}}}{\omega}} \approx 0.2\ \mu\mathrm{m}, \qquad \text{and} \qquad \delta = \sqrt{\frac{2\nu}{\omega}} \approx 0.6\ \mu\mathrm{m}. \tag{5}$$

The time average of the first-order fields are zero, so the acoustic radiation force $\boldsymbol{F}^{\mathrm{rad}}$ is the time average (angled brackets $\langle \dots \rangle$ below) of the second-order acoustic fields. The general expression for $\boldsymbol{F}^{\mathrm{rad}}$ is the following surface integral [3]

$$\boldsymbol{F}^{\mathrm{rad}} = \oint_{\mathrm{surf}} \big\langle \boldsymbol{\sigma}_2 - \rho_0\boldsymbol{v}_1\boldsymbol{v}_1\big\rangle\cdot\boldsymbol{n}\,\mathrm{d}a, \quad \text{(integral over the equilibrium surface of the sphere)}, \tag{6}$$

where $\boldsymbol{\sigma}_2$ is the stress tensor of the fluid to second order, and $\boldsymbol{n}$ is the outward surface normal vector.

Corresponding author. Henrik.Bruus@nanotech.dtu.dk
Supported by the Danish Council for Independent Research, Grant No. 274-09-0342.

RESULTS

The first-order scattering problem splits into a monopole term (the vibration of a stationary, compressible sphere) and a dipole term (the translation of a moving, rigid sphere). With this decomposition, the problem reduces to find the corresponding scattering coefficients, which then are inserted into expression (6) for $\boldsymbol{F}^{\mathrm{rad}}$. Some relevant parameters are $\tilde{\rho}$ (particle/fluid density ratio), $\tilde{\kappa}$ (particle/fluid compressibility ratio), $\tilde{\delta} = \delta/a$, $\tilde{\delta}_{\mathrm{th}} = \delta_{\mathrm{th}}/a$, and $ka = 2\pi a/\lambda$.

Fluids without thermal expansion. For a fluid without thermal expansion ($\alpha = 0, \gamma = 1$), the thermal and acoustic fields in Eq. (4) decouple, and $T_1 = 0$. The term $\langle \boldsymbol{\sigma}_2 \rangle$ in Eq. (6) is written as products of first-order fields, and by matching the first-order solutions for p_1 and $\boldsymbol{v}_1$ in the inviscid bulk with the those inside the boundary layer, we calculate $\boldsymbol{F}^{\mathrm{rad}}$ for arbitrary standing and traveling waves. For the special case of a planar standing wave, $p_{\mathrm{in}} = p_{\mathrm{a}} \cos(kz)$, we find

$$F^{\mathrm{rad}}_{\mathrm{1D}}(z) = 4\pi\left[\frac{f_1}{3} + \frac{f_2^{\mathrm{r}}}{2}\right] a^3 k E_{\mathrm{ac}} \sin(2kz), \quad f_1 = 1 - \tilde{\kappa}, \quad f_2^{\mathrm{r}} = \mathrm{Re}\left[\frac{2\big[1-\Gamma\big](\tilde{\rho}-1)}{2\tilde{\rho}+1-3\Gamma}\right], \quad \Gamma = -\frac{3}{2}\Big[1+\mathrm{i}(1+\tilde{\delta})\Big]\tilde{\delta}, \tag{7}$$

where E_{ac} is the acoustic energy density. The monopole scattering coefficient f_1 is unaffected by viscosity, but the dipole coefficient f_2^{r} depends on viscosity through the variable Γ. As in Doinikov [3], we have $ka \ll 1$ and $ka\tilde{\delta} \ll 1$ (the wavelength is the largest length scale in the problem), but in contrast to the previous result, we have no further restriction on $\tilde{\delta}$. In the limits $\tilde{\delta} \ll 1$ and $\tilde{\delta} \gg 1$, studied by Doinikov, his results and Eq. (7) agree. For near-neutral-buoyancy particles ($\tilde{\rho} \approx 1$), the influence of viscosity on the radiation force is negligible. For the often used polystyrene microbeads ($\rho_{\mathrm{ps}} = 1.05$ kg/m^3) in pure water, the relative change in the radiation force is 0.1 % for $a = 1$ µm and 0.2 % for $a = 0.1$ µm. For saltwater with a salinity (near saturation) of 25 % the effect increases due to increasing viscosity, and reaches 3 % for $a = 1$ µm and 5 % for $a = 0.1$ µm. For buoyant particles, e.g. pyrex glass with $\rho_{\mathrm{py}} = 2.23 \times 10^3$ kg/m^3, the influence of viscosity on the radiation force becomes important. We now find that in pure water the relative change in the radiation force is 15 % for $a = 1$ µm and 33 % for $a = 0.1$ µm. For saltwater with a salinity (near saturation) of 25 % the effect slightly decreases due to the lowering of $\tilde{\rho}$, and reaches 11 % for $a = 1$ µm and 22 % for $a = 0.1$ µm.

Fluids with thermal expansion. The analysis is more complicated when taking the volume thermal expansion into account ($\alpha > 0, \gamma > 1$). Space limitation prevents the full expressions to be given, so we restrict ourselves to the limit $\delta_{\mathrm{th}}, \delta \ll a \ll \lambda$, corresponding to the analysis provided by Doinikov. The expression for $F^{\mathrm{rad}}_{\mathrm{1D}}$ in this limit is

$$F^{\mathrm{rad}}_{\mathrm{1D,th}} = 4\pi\left[\frac{5\tilde{\rho} - 2 - \tilde{\kappa}}{3(2\tilde{\rho}+1)} + \frac{3(\tilde{\rho}-1)^2}{(2\tilde{\rho}+1)^2}\,\tilde{\delta} - \frac{\gamma - 1}{2(1+\tilde{\Delta})}\,\tilde{\delta}_{\mathrm{th}}\right] a^3 k E_{\mathrm{ac}} \sin(2kz), \tag{8}$$

where $\tilde{\Delta} = \tilde{\sigma}_{\mathrm{th}}/\sqrt{\tilde{D}_{\mathrm{th}}} \approx 1$ involves the particle/fluid ratios of the thermal conductivity $\tilde{\sigma}_{\mathrm{th}}$ and diffusivity $\tilde{D}_{\mathrm{th}}$. Above, we have seen how minute the changes are in the radiation force when only viscosity is taken into account. Thus, we measure the influence of the thermal effects by the ratio R of the thermal δ_{th}-term and the viscous δ-term in Eq. (8):

$$R = \frac{(\gamma-1)(2\tilde{\rho}+1)^2}{6(1+\tilde{\Delta})(\tilde{\rho}-1)^2}\sqrt{\frac{D_{\mathrm{th}}}{\nu}} \approx 3.1 \times 10^{-4}\,\frac{(2\tilde{\rho}+1)^2}{(\tilde{\rho}-1)^2}, \tag{9}$$

where the pre-factor is calculated for water. For neutral buoyancy ($\tilde{\rho} = 1$) the viscous term is zero and R is not defined. However, because $\gamma - 1 = 0.01$ and $\delta_{\mathrm{th}} = 0.4\delta$, the thermal effect is small ($\lesssim 1$ %). For the case of polystyrene, $\tilde{\rho} = 1.05$, we find that $R = 1.2$, and the viscous and thermal effect are of the same magnitude. However, as these two terms in Eq. (8) have opposite signs, they actually nearly cancel each other. For pyrex glass, $\tilde{\rho} = 2.23$, we obtain $R = 0.006$, and again the thermal effect is negligible. The same conclusion can be reached in the limit $\tilde{\rho} \to \infty$, because $R \to 1.2 \times 10^{-3}$.

CONCLUSIONS

Extending previous work by Doinikov [3], we have calculated the acoustic radiation force on a compressible, spherical micro-particle suspended in a viscous, thermal conducting fluid exposed to an ultrasound field. We have used the resulting expression to quantitatively analyze microchannel acoustophoresis, and found that for nearly-neutral-buoyancy particles, the effect of the viscosity on the radiation force disappears, while a small ($\lesssim 1$ %) thermal correction remains. For buoyant particles ($\tilde{\rho} > 1.05$) the effect of viscosity can be significant (larger than 30 %), but the thermal effect remains a small fraction of this ($R < 0.001$).

References

[1] J. Friend and L. Y. Yeo: Microscale acoustofluidics: Microfluidics driven via acoustics and ultrasonics. *Rev Mod Phys* **83**, 647–704 (2011).

[2] H. Bruus, J. Dual, J. Hawkes, M. Hill, T. Laurell, J. Nilsson, S. Radel, S. Sadhal and M. Wiklund: Forthcoming Lab on a Chip tutorial series on acoustofluidics: Acoustofluidics-exploiting ultrasonic standing wave forces and acoustic streaming in microfluidic systems for cell and particle manipulation. *Lab Chip* **11**, 3579–3580 (2011).

[3] A. A. Doinikov: Acoustic radiation force on a spherical particle in a viscous heat-conducting fluid . Part 1. General formula. *J Acoust Soc Am* **101**, 713–721 (1997). *Ibid*: Part 2. Force on a rigid sphere. *J Acoust Soc Am* **101**, 722–730 (1997).

[4] H. Bruus: Acoustofluidics 2: Perturbation theory and ultrasound resonance modes. *Lab Chip* **12**, 20–28 (2012).