Modelling acoustofluidic microdevices

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Numeric models simulating first order acoustic fields in a Newtonian fluid domain bounded by a solid and an actuating surface are presented. The numeric models are used to investigate boundary conditions commonly used in microfluidic simulations to model either pressure or velocity fields along fluid-solid interfaces. The conditions are; 1) The hard wall condition, used to model fluid-solid interfaces assumed to not yield due to fluid pressure. 2) The lossy wall condition, used to model fluid-solid interfaces that yield, based on the relation between the fluid and solid acoustic impedances. By comparing the acoustic fields resulting from simulations coupling linear elasticity and fluid dynamics along interfaces, with simulations relying solely on fluid dynamics and aforementioned approximate boundary condition along boundaries, the validity of said approximations can be investigated.

I. INTRODUCTION

With the advent of acoustophoresis as a particle separation technique, exact modelling of acoustofluidic microdevices is of increasing importance to optimise device design. In the literature, microdevice modelling is often performed using boundary condition simplifications of the interaction between microchannel wall and device [1, 2], to exclude the microchannel from simulations. Depending on chip geometry, material, and actuation parameters this may be a reasonable approximation in some cases, but as we will show, this is generally not the case.

II. THEORY

A numeric model is set up in COMSOL Multiphysics. The model consists of a fluid domain bounded to the sides and upwards by a solid domain as shown in Fig. 1. Both domains are bounded downwards by a piezoelectric substrate, which in the model is replaced by a boundary condition. Additionally, a reduced version of the model is generated in which the interaction of fluid and solid along interfaces are replaced by boundary conditions.

In the fluid domain of the model, the governing equations are first-order mass and momentum conservation, with temperature assumed constant - Eqs. (1a) and (1b) - as found using perturbation theory [3].

$$\partial_t p_1 = -\rho_0 c_0^2 \boldsymbol{\nabla}\cdot\boldsymbol{v}_1 \tag{1a}$$

$$\rho_0 \partial_t \boldsymbol{v}_1 = \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_1 \tag{1b}$$

where ∂_t is the time derivative, p_1 is the first order pressure, ρ_0 is the initial density, c_0 is the initial sound velocity, $\boldsymbol{v}_1$ is the first order velocity vector, and $\boldsymbol{\sigma}_1$ is the first order stress tensor.

In the solid material, linear elasticity is applied, as only small perturbations are assumed.

$$\rho_s {\partial_t}^2 \boldsymbol{u}_\mathrm{s} = \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_\mathrm{s}\,, \tag{2}$$

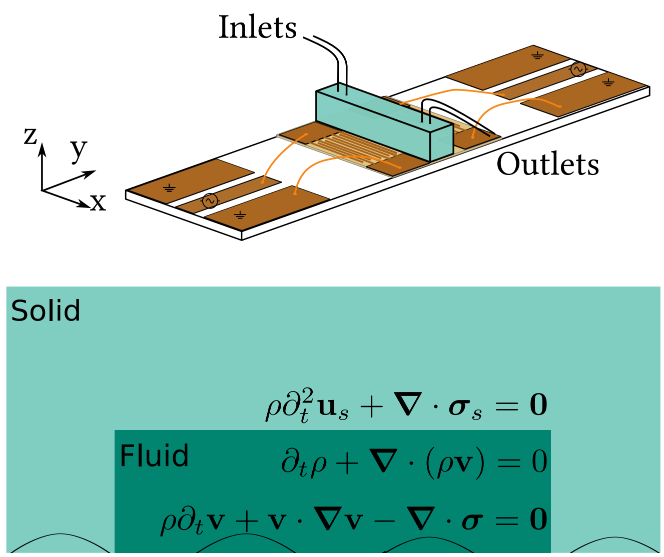

FIG. 1. Basis of work. (above) The numeric model is based on an acoustofluidic device experimented on at the Microfluidics group at NTNU. (below) The model consists of two separate domains, a fluid domain governed by Navier-Stokes and a solid domain governed by linear elasticity. The two domains are actuated by a piezoelectric substrate, which in the model is simplified through an analytical, harmonic expression. The model can be reduced further, to consist solely of a fluid domain. The effects of this simplification is the focus of this study.

where ρ_s is the solid density, $\boldsymbol{u}_\mathrm{s}$ is the displacement vector, and $\boldsymbol{\sigma}_\mathrm{s}$ is the solid stress tensor.

In order to couple the fluid and solid motions, the motion in the fluid along the wall is determined by the motion of the solid, while the stress in the solid along the same interface is determined by the stress in the fluid as shown in Eq. (3).

$$\boldsymbol{v} = \partial_t \boldsymbol{u}_s = -i\omega \boldsymbol{u}_s \tag{3a}$$

$$,\boldsymbol{n}_s\cdot\boldsymbol{\sigma}_s = \boldsymbol{n}_s\cdot\boldsymbol{\sigma}_f\,. \tag{3b}$$

As mentioned, an analytical expression is imposed as a boundary conditions along the lower boundary of the system to emulate the motion of the piezoelectric substrate.

$$\boldsymbol{v} = \partial_t \boldsymbol{u}_{pz} = -i\omega \boldsymbol{u}_{pz} \tag{4a}$$

$$, \boldsymbol{u}_s = \boldsymbol{u}_{pz} \,, \tag{4b}$$

Including the solid surrounding the fluid in numerical models can be computationally heavy - and give rise to numerical difficulties for some materials. Hence, many numerical models in the literature solely model the fluid domain and replace the coupling outlined above with boundary conditions, to emulate the interactions. Depending on the interfacing material one of two boundary conditions are usually applied; hard wall or lossy wall, as shown in Eqs. (5) and (6) [3].

The boundary conditions imposed, are designed to approximate different materials. The hard wall condition Eq. (5) is intended to approximate hard materials, e.g. borosilicate glasss by assuming the material does not move at all, i.e. the velocity of the fluid along the interface is fixed,

$$\boldsymbol{n} \cdot \boldsymbol{v}_1 = 0 \quad \text{or} \quad \boldsymbol{n} \cdot \boldsymbol{\nabla} p_1 = 0 \,. \tag{5}$$

The lossy wall condition Eq. (6) approximates a wall through which there are radiative acoustic losses. The condition approximates wall motion based on the fluid pressure and the acoustic impedance of the surrounding material;

$$\boldsymbol{n} \cdot \boldsymbol{v}_1 = \frac{1}{\rho_s c_s} p_1 \quad \text{or} \quad \boldsymbol{n} \cdot \boldsymbol{\nabla} p_1 = \frac{i\rho_0 \omega}{c_s \rho_s} p_1 \,. \tag{6}$$

To carry out analysis of the imposed conditions, the acoustic fields resulting from models using boundary conditions are compared to the acoustic fields found when including the surrounding material in simulations. Similarities between these results would indicate a good approximation, while deviations indicate that the conditions are not representative.

III. RESULTS

The hard wall was found to be a reasonable approximation to obtain an idea of acoustic fields within a fluid bounded by borosilicate glass, if the thickness was 1500 or above. The appearance of acoustic fields could be well approximated at lower thicknesses when actuated at a resonant frequency. However, if exact values are needed, the entire system ought to be modelled, as these depends on system resonance, and the hard wall may over- or underestimate the actual value. This was supported by the comparison between imposed conditions and actual conditions, for which resonance of the solid structure comes into play.

[1] N. Nama, R. Barnkob, Z. Mao, C. J. Kähler, F. Costanzo, and T. J. Huang, Lab Chip **15**, 2700 (2015).

[2] K. Lee, H. Shao, R. Weissleder, and H. Lee, ACS Nano **9**, 2321 (2015).

[3] H. Bruus, Lab Chip **12**, 20 (2012).