Supplemental material for:
Theory and modeling of nonperturbative effects at high acoustic energy densities in thermoviscous acoustofluidics

Jonas Helboe Joergensen* and Henrik Bruus†
Department of Physics, Technical University of Denmark,
DTU Physics Building 309, DK-2800 Kongens Lyngby, Denmark
(Dated: 20 December 2022)

This supplemental material provides details the numerical model used in the 3D example in section VI-B in the main article.

The numerical model is the iterative and effective thermoviscous pressure acoustic model presented in the main paper with heating from an external LED. The model is an iterative model that solves the steady fields temperature field T_0 in the fluid and solid and the steady velocity $\boldsymbol{v}_0$ and pressure p_0 in fluid and the acoustic time-varying pressure p_1 in the fluid and displacement $\boldsymbol{u}_1$ in the solid. The model of a glass-silicon-glass chip with a fluid channel of height $H = 360$ µm and width $W = 760$ µm is shown in Fig. S1. In the model we take advantage of the symmetries in the system and model a quarter of the channel, Fig. S1. In the y-z symmetry plane at $x = 0$ all fields are symmetric, and in the x-z symmetry plane at $y = 0$ the acoustic fields p_1 and $\boldsymbol{u}_1$ are anti-symmetric and the stationary fields T_0, $\boldsymbol{v}_0$, and p_0 are symmetric. The model parameters are listed in Table S1.

The actuation is modeled not as a full piezoelectric transducer as in Ref. [1], but merely as a boundary condition with a displacement $d_0 = 5$ nm and a frequency f_0 on the black actuation plane in Fig. S1 as in Ref. [2]. Note that using the symmetry planes, the model actually has anti-symmetric actuation regions, one on each side of the chip.

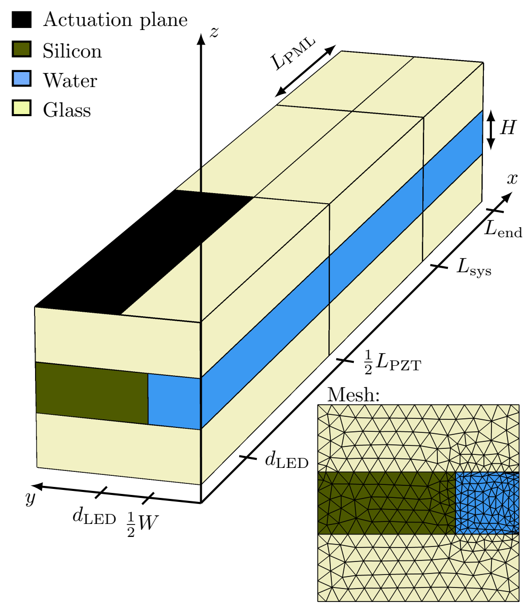

FIG. S1. Sketch of the numerical model of the acoustofluidic chip. Symmetry planes have been used so only a quarter of the channel is simulated. The model consists of a fluid domain with width W and height H, a solid domain (glass and silicon), and a special PML (perfectly matched layer) region where the travelling waves are artificially damped to mimic an infinitely long channel. The acoustic actuation is done on the actuation region (black) and the LED has its center at $x = 0$ and $y = 0$ and has half of the width d_{LED}. The mesh is shown in the y-z plane, which is swept along the x-axis so that the mesh node repeats itself with a distance of 51 µm.

TABLE S1. System parameters characterizing the geometry, the acoustic actuation, and the absorption of the LED spot.

Parameter	Symbol	Value	Unit
Geometry parameters:			
Fluid width	W	760	µm
Fluid height	H	360	µm
Actuation length	L_{PZT}	2.0	mm
System length	L_{sys}	4.0	mm
PML length	L_{PML}	1.75	mm
Total length	L_{end}	5.75	mm
Actuation parameters:			
Actuation amplitude	d_0	5.0	nm
Actuation frequency	f_0	0.957	MHz
LED parameters:			
Half width of the LED spot	d_{LED}	850	µm
Absorption coefficient	α	12.3	mm^{-1}

During operation, a piezoelectric transducer generates heat, but this is neglected in the simulations for two reasons: (1) The necessary acoustic energy density is obtained in the system using a relatively low power consumption, and this assures that the heat generation is relatively small. (2) The heat from the transducer is lead through the top glass layer into the silicon layer, where it due to the high heat conductivity of silicon is uniformly distributed throughout the chip, leading to only a minute and nearly uniform temperature rise in the microchannel.

To avoid simulating the entire chip, the perfectly matched layer (PML) method is used to artificially damp

* jonashj@fysik.dtu.dk
† bruus@fysik.dtu.dk

travelling waves [3]. Thus, the model consists of an area of length L_{PZT} where a piezoelectric transducer actuates the chip at a frequency f_0 with an amplitude d_0, a part of length $L_{\mathrm{sys}} - L_{\mathrm{PZT}}$ where there are no actuation, and finally a section of length L_{PML} where the acoustic waves are artificially damped using a PML. For the PML to be valid, the distance $L_{\mathrm{sys}} - L_{\mathrm{PZT}}$ must be long enough for the travelling wave to develop so that the acoustic field does not depend on where the PML starts.

The real device has a long channel with a long piezoelectric transducer. To model the pressure field around the LED spot accurately, the length L_{PZT} must be larger than half of the LED spot width d_{LED}. The LED spot is modeled as a Gaussian beam with half of the beam width $d_{\mathrm{LED}} = 850$ µm,

$$I(x, y, z) = \frac{2P_{\mathrm{LED}}}{\pi d_{\mathrm{LED}}^2} \exp\left[-\frac{2(x^2+y^2)}{d_{\mathrm{LED}}^2} - \alpha\Big(z + \frac{1}{2}H\Big)\right], \tag{S1}$$

where P_{LED} is the total power of the LED and $-\frac{1}{2}H$ is the bottom of the channel where beam starts to be absorbed. In the solution, the heat absorption is given as $q(x, y, z) = \alpha I(x, y, z)$ for $-\frac{1}{2}H < z < \frac{1}{2}H$, while the absorption in the glass is neglected.

The entire model is implemented in COMSOL Multiphysics 5.6, with the governing equations and effective boundary conditions given in the main article. The numerical model uses cubic test functions for the streaming field and the acoustic pressure field, but quadratic test functions for the acoustic displacement field in the solid and the second-order pressure field.

[1] N. R. Skov, J. S. Bach, B. G. Winckelmann, and H. Bruus, 3D modeling of acoustofluidics in a liquid-filled cavity including streaming, viscous boundary layers, surrounding solids, and a piezoelectric transducer, AIMS Mathematics **4**, 99 (2019).

[2] M. W. H. Ley and H. Bruus, Three-dimensional numerical modeling of acoustic trapping in glass capillaries, Phys. Rev. Appl. **8**, 024020 (2017).

[3] A. Bermúdez, L. Hervella-Nieto, A. Prieto, and R. Rodríguez, An optimal perfectly matched layer with unbounded absorbing function for time-harmonic acoustic scattering problems, J. Comput. Phys. **223**, 469 (2007).