Ultrasound-assisted Microfluidic Devices: Insights and Optimization of Sono-Microreactors

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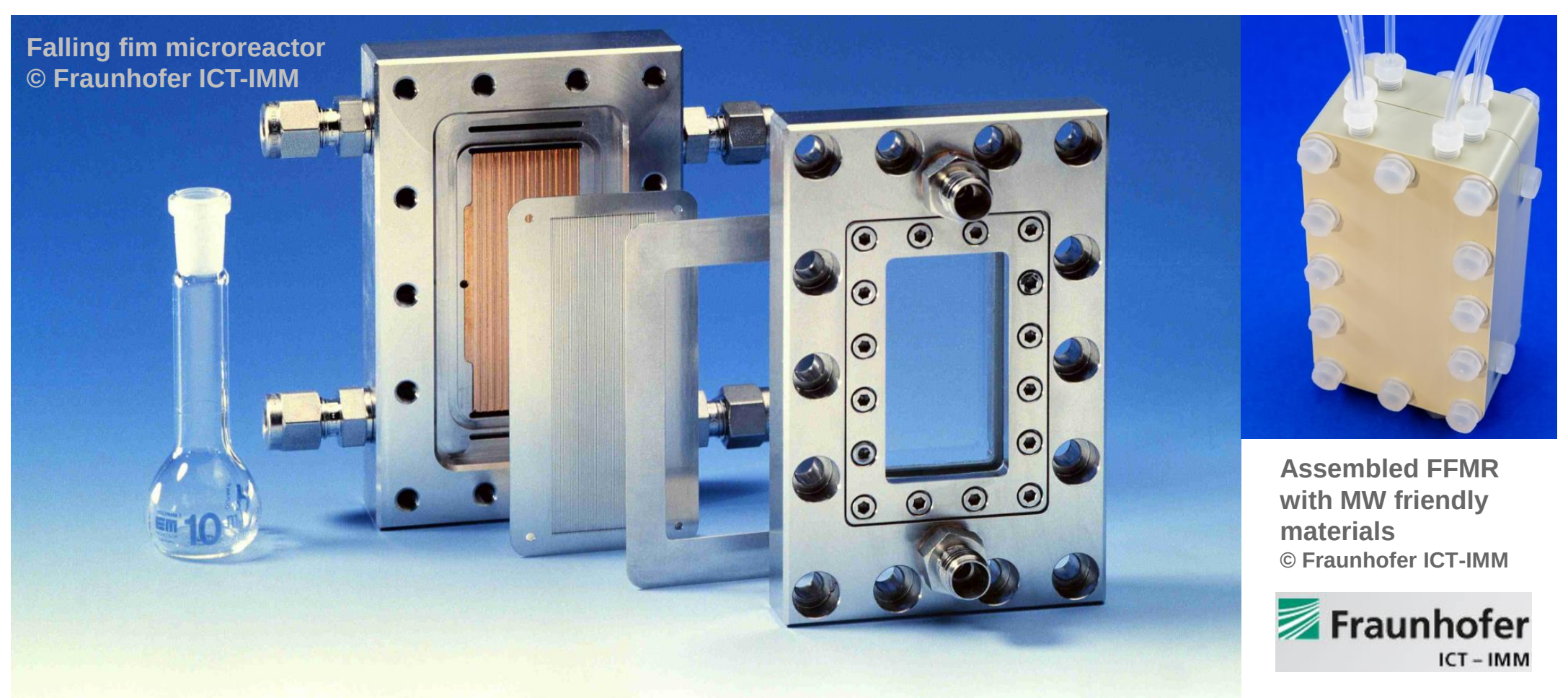
Microfluidic devices, also known as Lab on a Chip, are currently facing an increasing demand, especially in the fine chemistry sector and, more specifically, in the pharmaceutical and food industry. The use of these microreactors leads to green and economical production methods due to a higher selectivity of target products and reduced waste. Ultrasonic irradiation has been successfully implemented for preventing clogging in microreactor configurations, ranging from capillaries immersed in ultrasonic baths to devices with miniaturized piezoelectric transducers. Moving forward in process intensification and sustainable development, the acoustic energy implementation requires a strategy to optimize the microreactor from the ultrasonic viewpoint during its design. This can be achieved with appropriate modeling through finite element methods.

Introduction to microfluidics



Microfluidic devices (a.k.a. *Lab on a Chip*) enable a convenient manipulation of chemical reactions by reducing the diameter of the reactor channels to tens/hundreds of micrometres. The use of small quantities of reagents and solvents leads to ***green*** production methods if one considers the high selectivity and reduced amount of waste.

The usual workflow to optimize the benefits of US within microreactors is by changing the applied frequency once the device is mounted.

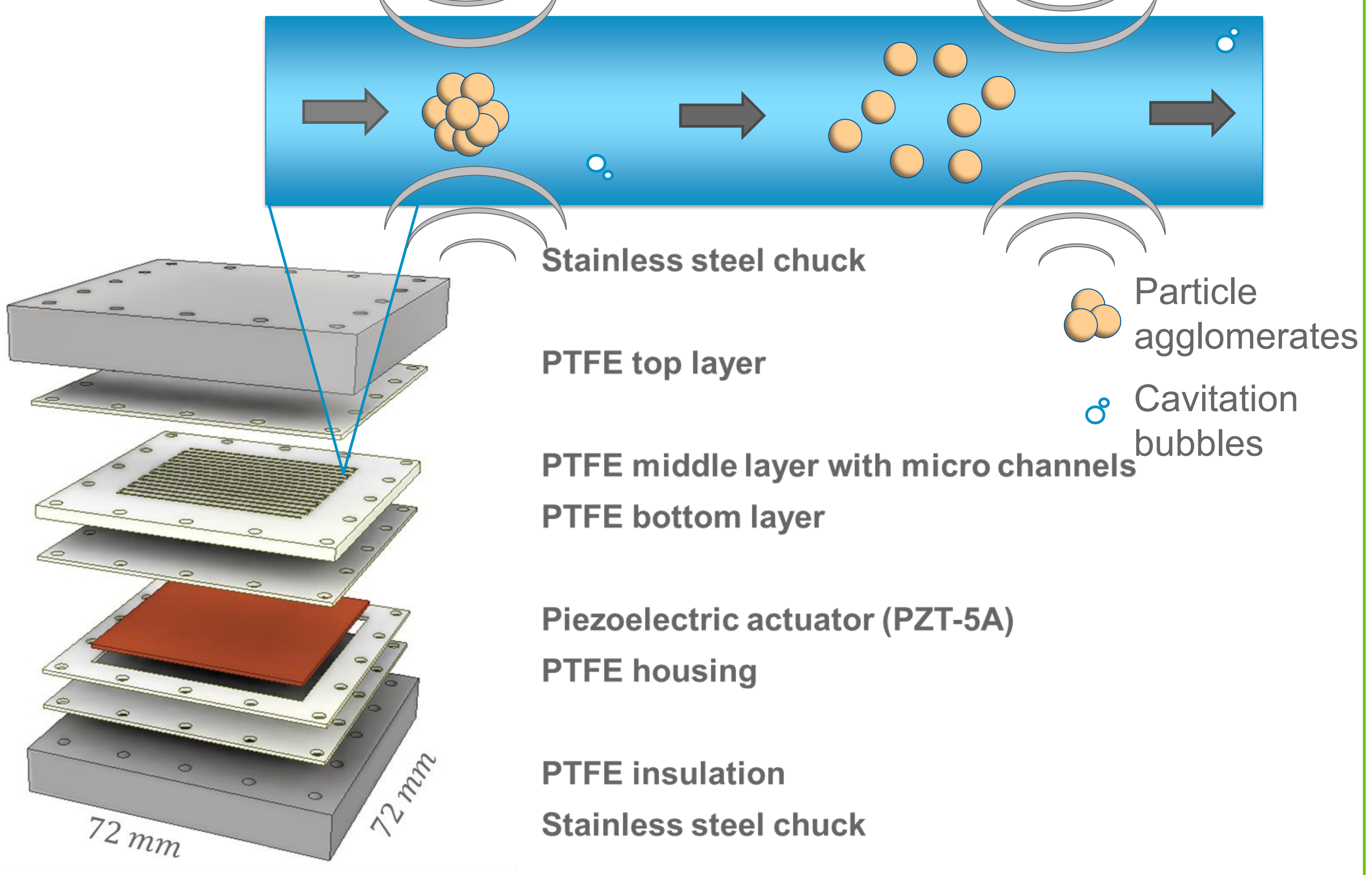
Why ultrasound?

Acoustic intensification is being applied to microreactors in different forms and with different sizes and geometries.[1]

Effects:

- **Cavitation**
  - Acoustic streaming
  - Micro-jetting
  - Shock waves
- Improvement of mass transport
- Surface cleaning
- Sonoluminescence
- Chemical effects

Ultrasound irradiation prevents microchannel clogging



Representation of the assembly constituting the Teflon-stacked microreactor proposed by Kuhn et al.[2]

One-dimensional: Langevin Equation

Backing design

$$k_p l_p + tan^{-1}\left(\frac{Z_b}{Z_p}\tan k_b l_b\right) = \frac{\pi}{2}$$

Matching design

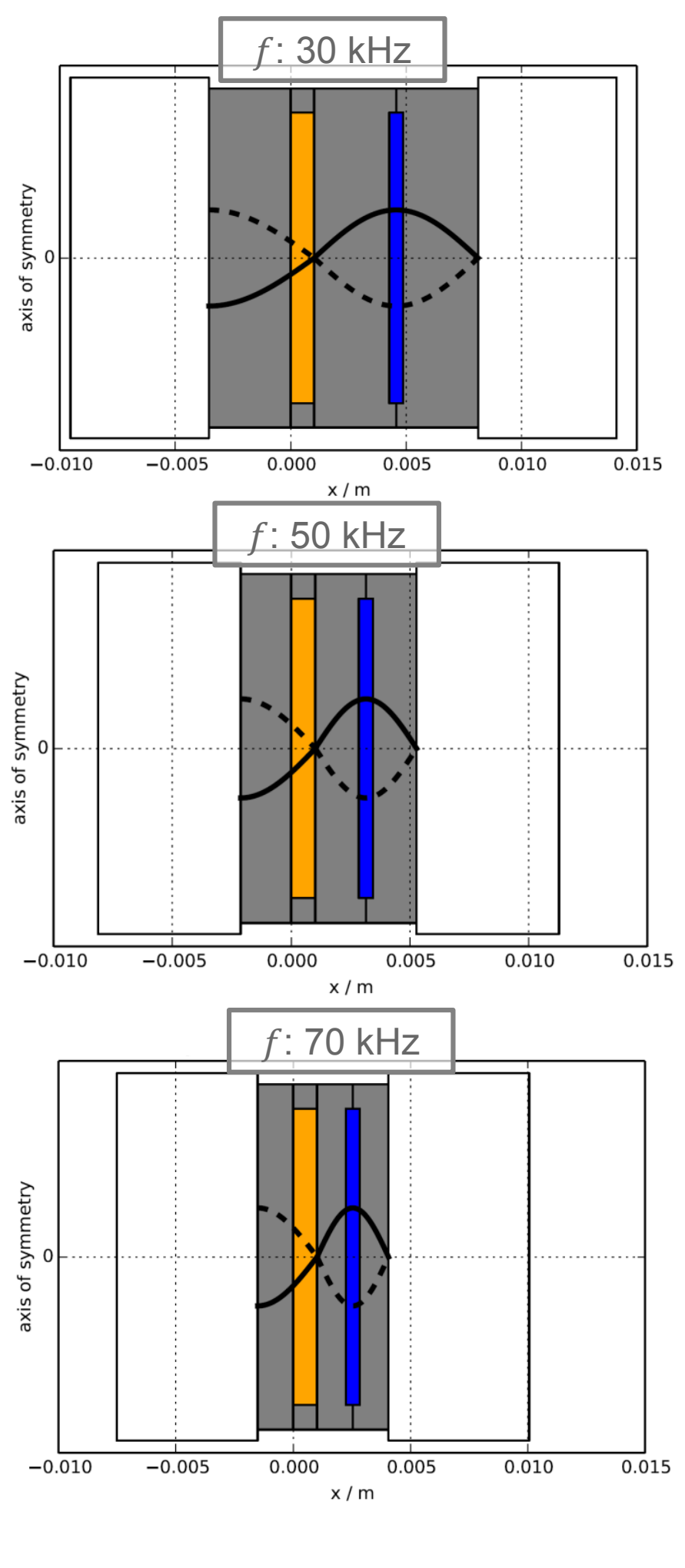
$$tan^{-1}\left(\frac{Z_f}{Z_p}\tan k_f l_f\right) = \frac{\pi}{2}$$

l_p: thickness of the PZT
l_b: thicknesses of the Teflon (back)
l_f: thicknesses of the Teflon (front)
k: angular wavenumber ($2\pi f / v_p$)
$Z = \rho c$: acoustic impedance

▨ PTFE
🟧 PZT
🟦 Water
☐ St. Steel

— Displacement (u)

Sizing according to Langevin Equation:

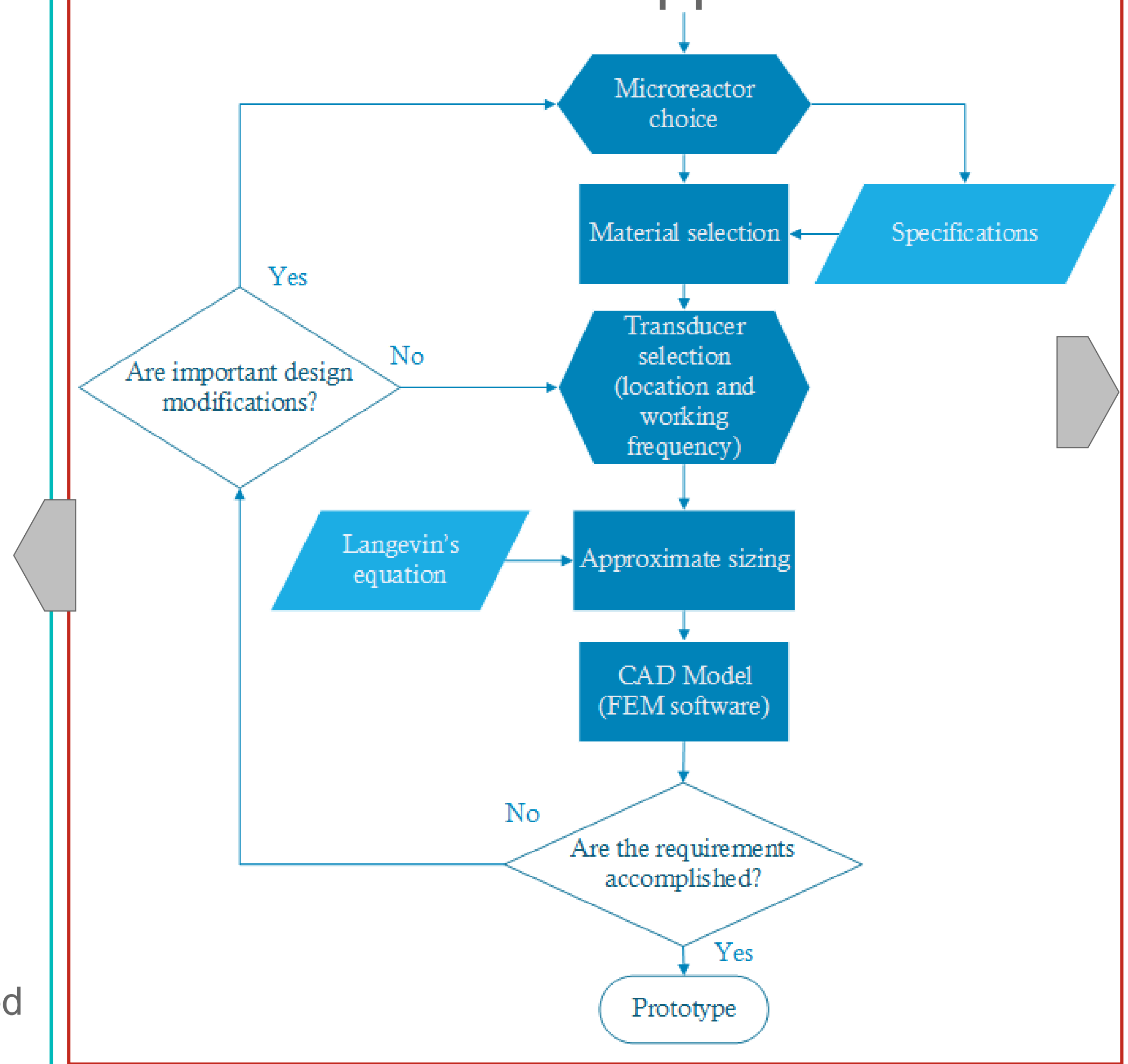


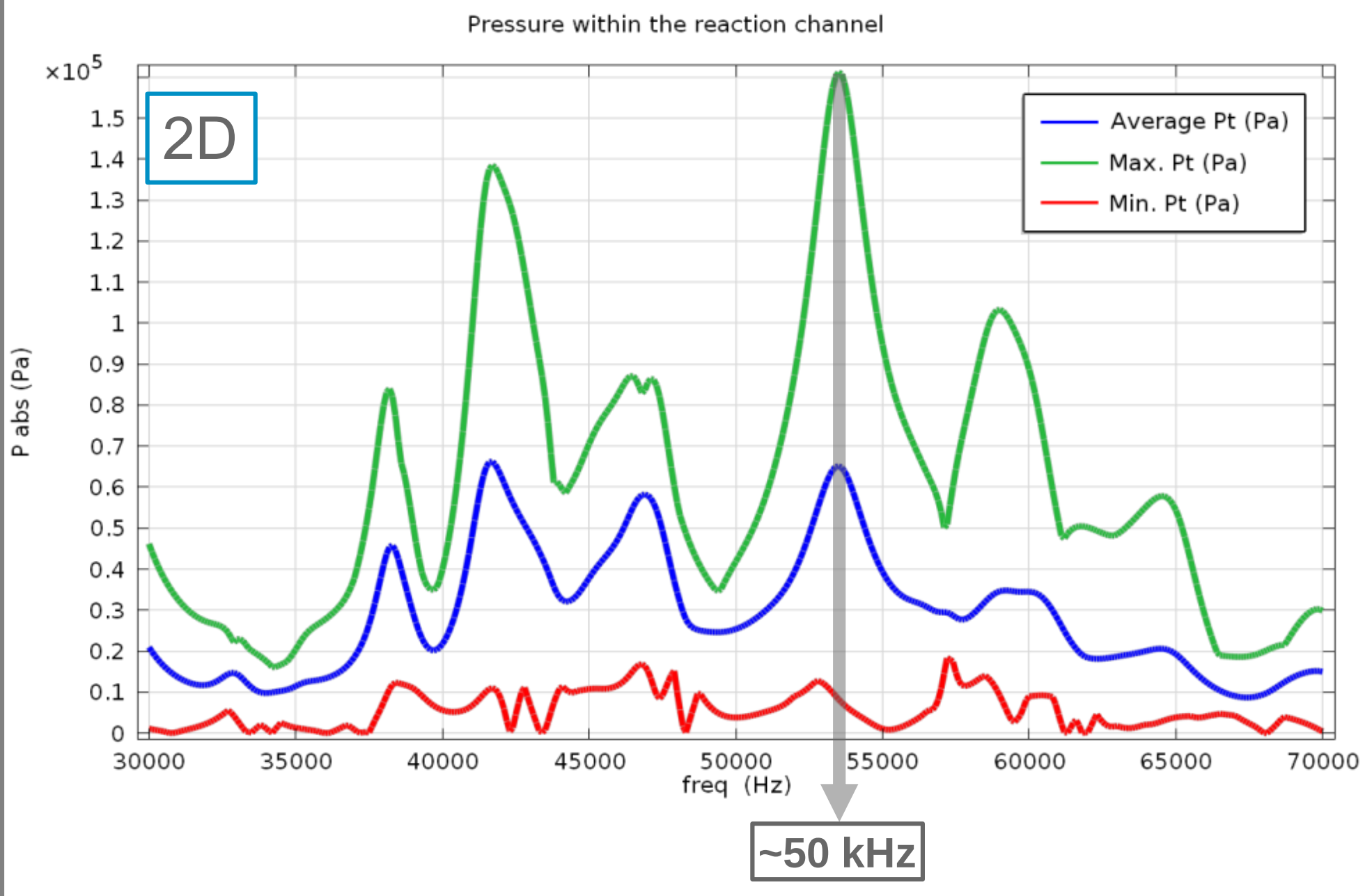
Langevin equation[3,4] solved at 50 kHz provides similar dimensions as the microreactor described in the literature.

50 kHz

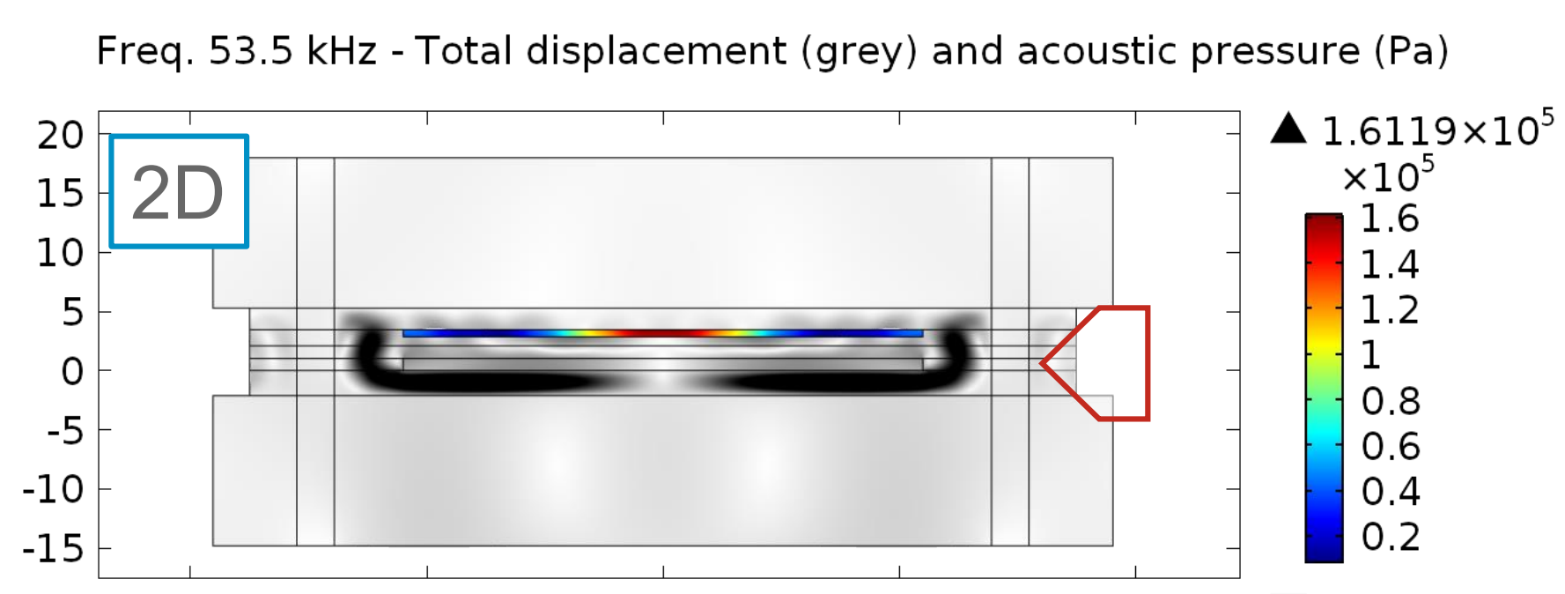
A prototype including these calculated dimensions has been numerically tested by using Finite Element Method (FEM) simulations.

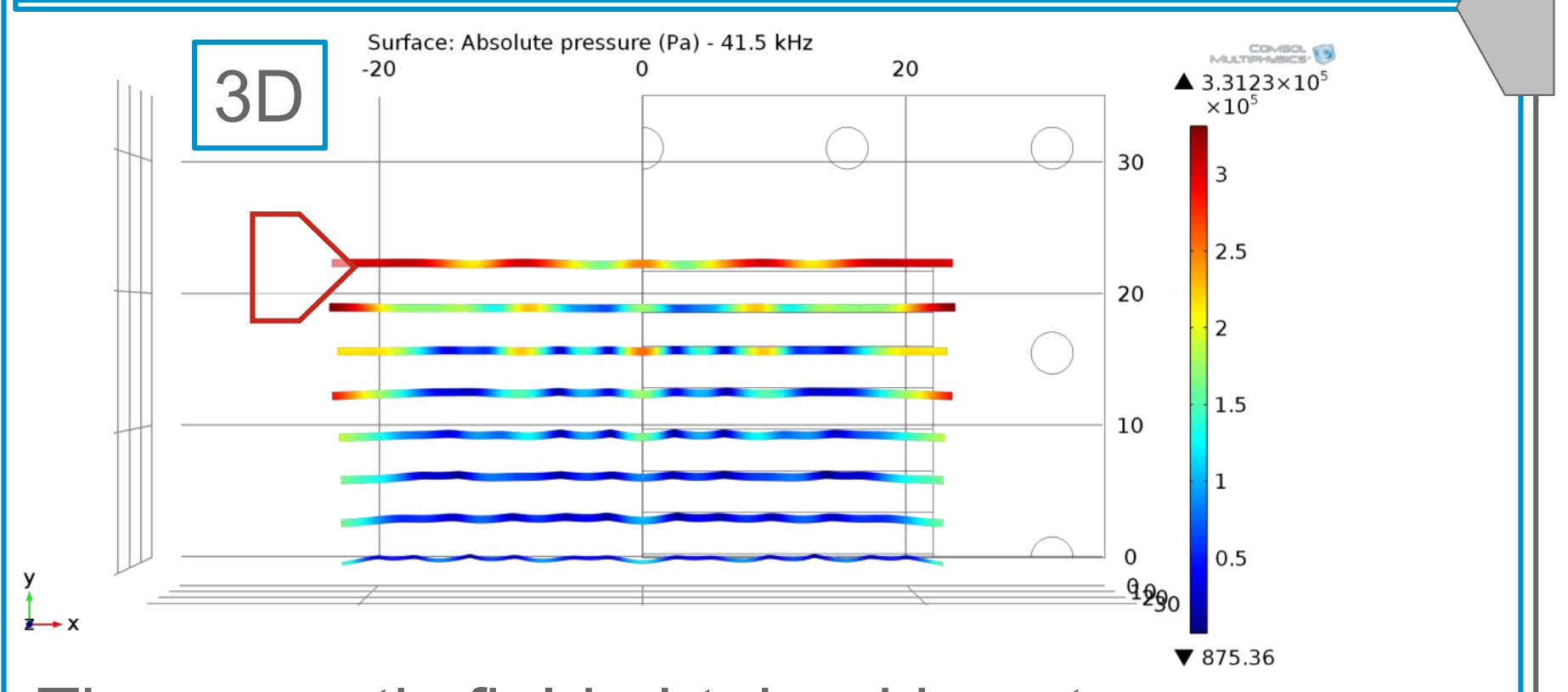
Modeling scheme: An alternative approach



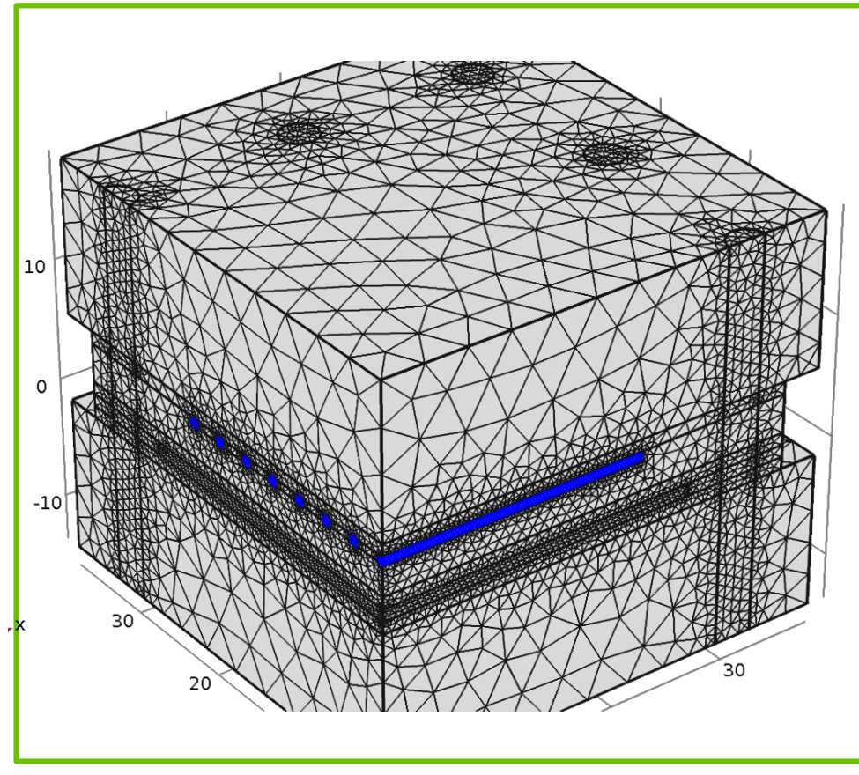


A 2D model allows us to explain the experimental observations where best results were obtained at 50kHz



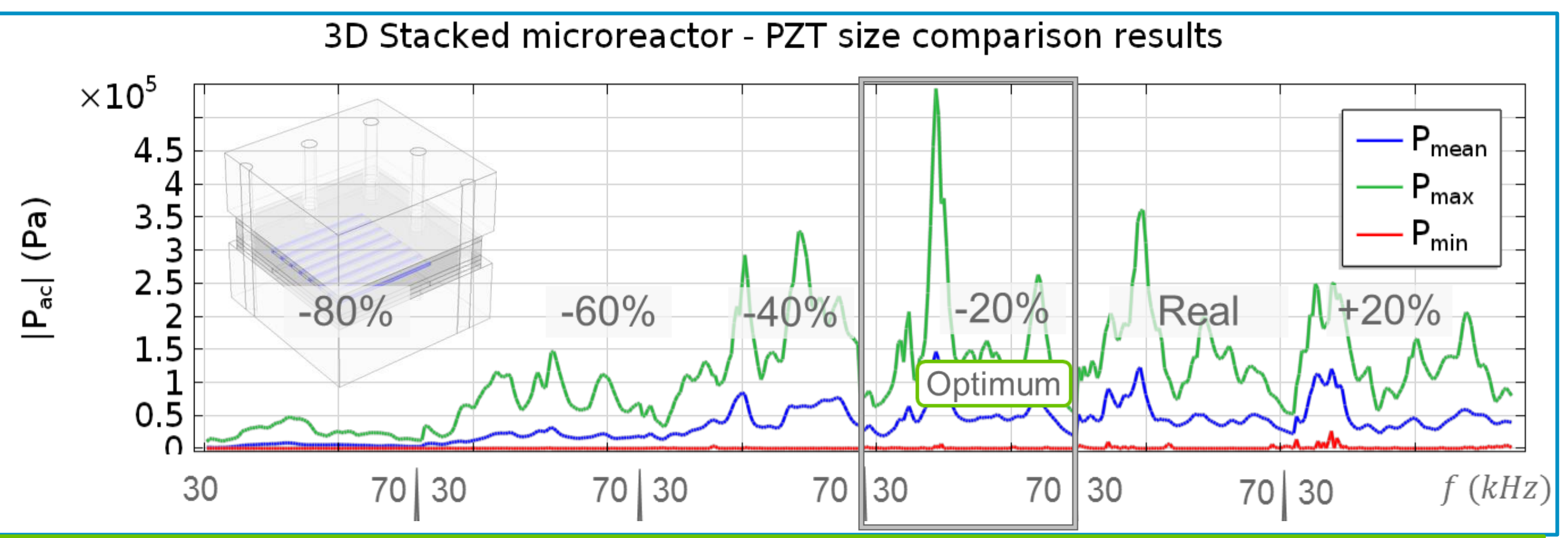


The acoustic field obtained is not homogeneous. Simulation provides insights on the effects of geometry an materials used.



Several 3D prototypes have been tested varying the length of the PZT among other parameters. The liquid and the actuator domain required a finer mesh in order to show consistent results.

A frequency sweep (30-70kHz) for each size of the PZT can shown how a reduction of 20% increases the acoustic pressure obtained. Consequently, PZT material and energy consumption can be reduced.



Numerical model: Governing equations

- Linear Acoustics in the working liquid

$$\nabla^2 p + \left(\frac{\omega}{c}\right)^2 p = 0$$

Helmholtz equation

p: the acoustic pressure
c: speed of sound in the liquid
ω: angular frequency

- Vibration of the solid

Linear elastic and isotropic solid materials

$$-\rho_s \omega^2 \mathbf{u} = \nabla\sigma\ ,\ \sigma = \boldsymbol{s}$$

$$\boldsymbol{s} = \frac{E\nu}{(1+\nu)(1-2\nu)}(\mathrm{Tr}\boldsymbol{\varepsilon})\boldsymbol{I} + \frac{E}{1+\nu}\boldsymbol{\varepsilon}$$

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)$$

ρ_s: density of the solid
$\boldsymbol{u}$: displacement field
$\sigma = \boldsymbol{s}$: elastic strain tensor
E: Young's modulus
ν: Poisson's ratio
$\boldsymbol{I}$: Identity Tensor
Tr: trace operator
$\boldsymbol{\varepsilon}$: total strain tensor

- Piezoelectric material (stress-charge form)

$$\boldsymbol{\sigma} = c_E\varepsilon - e^T\boldsymbol{E}$$

$$\boldsymbol{D} = e\varepsilon + \epsilon_s\boldsymbol{E}$$

c_E: elasticity matrix
e: coupling matrix
$\boldsymbol{E} = -\nabla V$: electric field
$\boldsymbol{D}$: electric displacement field
ϵ_s: permittivity matrix

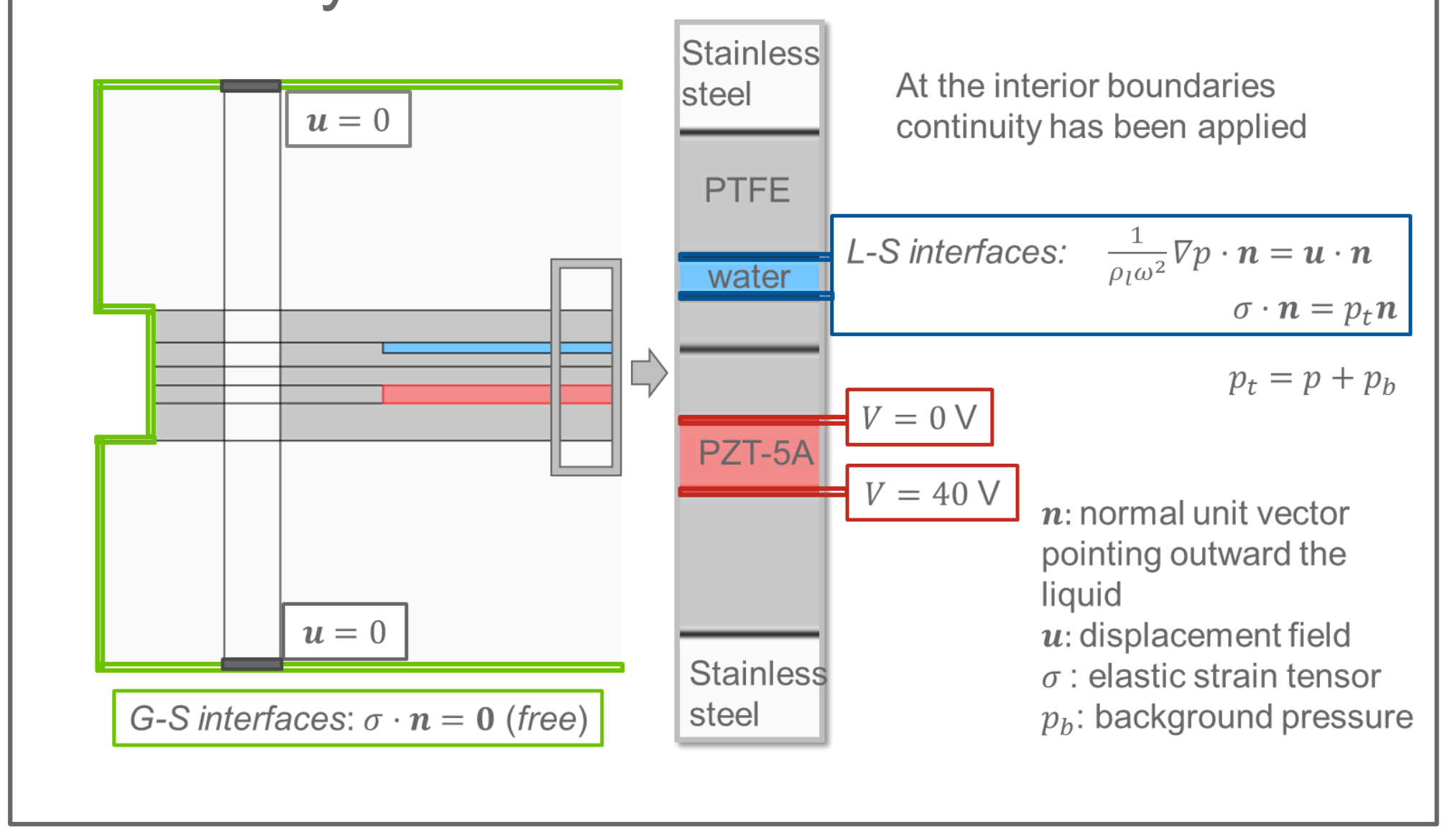
- Damping

Viscoelastic materials

$$E(T,f) = E_1 + iE_2 = E_1(1 + i\eta)$$

E_1: Young's storage modulus
E_2: Loss modulus
$\eta = \frac{E_2}{E_1}$: Isotropic loss factor

Boundary conditions



At the interior boundaries continuity has been applied

L-S interfaces: $\frac{1}{\rho_l\omega^2}\nabla p \cdot \boldsymbol{n} = \boldsymbol{u}\cdot\boldsymbol{n}$, $\sigma\cdot\boldsymbol{n} = p_t\boldsymbol{n}$

$p_t = p + p_b$

G-S interfaces: $\sigma\cdot\boldsymbol{n} = \boldsymbol{0}$ *(free)*

$\boldsymbol{n}$: normal unit vector pointing outward the liquid
$\boldsymbol{u}$: displacement field
σ : elastic strain tensor
p_b: background pressure

CONCLUSIONS

- The incorporation of ultrasound irradiation offers potential advantages for preventing microreactor-related problems and enhancing their performance.
- Analytical models give an idea of the dimensions of the backing and matching elements in contact with the piezoelectric actuator for achieving resonance.
- Numerical simulations can help both rationalize the experimental results and gain insights into the physics involved in sono-microreactors which can lead ultimately to optimized devices
- Further work is underway to extend the acoustic simulation by involving several multiphysics phenomena such as fluid dynamics and chemical reaction.

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