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

F. J. Navarro-Brull[1], P. Poveda[2], J. Ramis[2], R. Gómez[1]

[1]Departament de Química Física, Universidad de Alicante, Alicante, Spain
[2]Departament de Física, Enginyeria de Sistemes i Teoria del Senyal, Universidad de Alicante, Alicante, Spain

Abstract

Microfluidic devices, also known as Lab on a Chip, are currently facing an increasing demand especially in the fine chemistry sector such as pharmaceutical or food industry. They can exhibit significant advantages over classical reactors because the reaction conditions in the microchannels noticeably differ from those in large-scale reactors. However, possible drawbacks of microreactors are inefficient reactant mixing due to the predominance of laminar flow and clogging (when solid-forming reactions are performed or solid catalyst suspensions are used).

The use of ultrasonic irradiation has been successfully implemented not only to prevent these problems because of its well-known mixing and particle-dispersion effects, but also because of mass transport enhancement or potential solid catalyst reactivation. Several configurations have been used for this purpose ranging from immersion of the capillaries in ultrasonic baths or cavitation tubes (Figure 1), to the integration of miniaturized piezoelectric transducers in the microchannel plate (Figure 2).
The acoustic field generated in the microreactor strongly depends on its configuration —i.e. working frequency of the transducer, construction materials, sizes and geometries of the different parts, etc.—. The complexity that ultrasonic irradiation and its optimization involve is usually not regarded as determinant since its effects are a tool, not an end. For instance, the usual workflow to optimize the benefits of US within microreactors is by changing the applied frequency once the device is mounted. However, ultrasound irradiation (i.e. sonication) involves several physicochemical effects, many of them related to cavitation collapse and associated phenomena —e.g. sono-luminescence—, which strongly depend on the working frequency of the transducer. Consequently, a physical understanding of all these variables and their influence should be taken into account when optimizing the effects of ultrasound.

Numerical simulations can help both rationalize the experimental results and gain insights into the physics involved in sono-microreactors. By means of COMSOL Multiphysics® software, 3D simulations can be carried out to model the acoustic field inside the reactor, the vibrations of the solid, the acoustic pressure in the fluid and the electro-mechanical properties of the transducer. We have visualized and simulated the performance of several sono-microdevices found in the literature. Our research initial findings demonstrate that there is plenty of room for improvement in

this regard. For example, some authors just increased the number of transducers around the microfluidic device (Figure 2 and 3) in order to intensify the acoustic pressure generated. Empirical optimization of the working frequency and actuator/s location and size is not straightforward since vibrations can eliminate each other or produce a non-expected uneven pressure fields. Using COMSOL Multiphysics, we can evaluate these designs, perform a sensitivity analysis and truly understand the physics behind in order to optimize and propose new prototypes (Figure 4). As a result, improved designs of sono-microreactors could ultimately expand the possibilities that microfluidics devices are offering to fine chemical industries.

Reference

D., Fernandez Rivas et al., “Merging microfluidics and sonochemistry: towards greener and more efficient micro-sono-reactors.,” Chem. Commun. (Camb)., vol. 48, no. 89, pp. 10935 –47(2012)

J., Sedelmeier et al., “KMnO4-Mediated Oxidation as a Continuous Flow Process,” Org. Lett., vol. 12, no. 16, pp. 3618–3621(2010)
R. L., Hartman et al., “Overcoming the Challenges of Solid Bridging and Constriction during Pd-Catalyzed C - N Bond Formation in Microreactors Abstract: We investigate the mechanisms that govern plugging in microre-,” no. 12, pp. 1347–1357(2010)

S., Kuhn et al., “A Teflon microreactor with integrated piezoelectric actuator to handle solid forming reactions,” Lab Chip, vol. 11, no. 15, p. 2488(2011)

F., Castro et al., “Continuous-flow precipitation of hydroxyapatite in ultrasonic microsystems,” Chem. Eng. J., vol. 215–216, pp. 979–987(2013)
S., Aljbour et al., “Ultrasound-assisted capillary microreactor for aqueous–organic multiphase reactions,” J. Ind. Eng. Chem., vol. 15, no. 6, pp. 829–834(2009)

Y., Iida et al., “Ultrasonic cavitation in microspace,” Chem. Commun., no. 20, p. 2280(2004)
T., Tandiono et al. “Creation of cavitation activity in a microfluidic device through acoustically driven capillary waves.,” Lab Chip, vol. 10, no. 14, pp. 1848–55(2010)

T., Tandiono et al., “Sonolysis of Escherichia coli and Pichia pastoris in microfluidics,” Lab Chip, vol. 12, no. 4, pp. 780–786(2012)

C.L., Lee et al. “Enhancement of Nucleophilic Aromatic Substitutions by the Synergistic Effects of Microcavitation and Continuous-Flow Chemistry,” J. Flow Chem., vol. 3, no. 4, pp. 114 –117(2013)

F.J., Navarro-Brull et al., “Guidelines for the design of efficient sono-microreactors ,” Green Processing and Synthesis , vol. 3 . p. 311(2014)

Figures used in the abstract

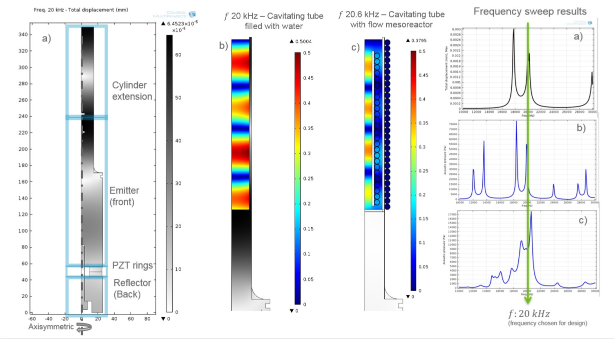

Figure 1: A ultrasonic horn (a) is simulated and also validated by reproducing and rationalizing its manufactured working frequency (20 kHz). The acoustic pressure distribution in a liquid cavitation tube (b) shows the impact that the geometry has over the tubing forming the meso-reactor (c).

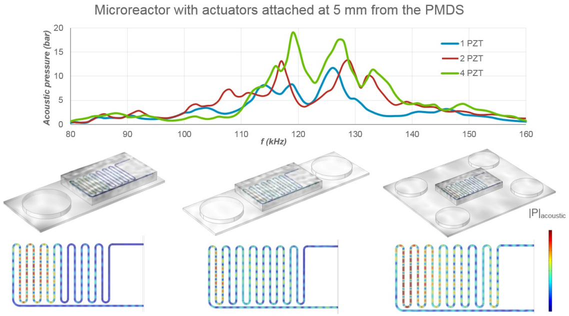

Figure 2: Acoustic pressure level within the liquid in the microchannel for a PDMS microfluidic device with different attached PZT transducer configurations as a function of the frequency. Contrary to the strategies found in the literature, the addition of more actuators does not always produce a more intense acoustic cavitation.

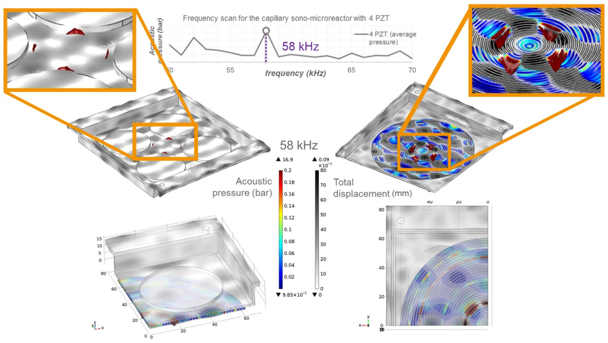

Figure 3: Acoustic simulations showed optimum resonance frequencies (58 kHz) very close to that used by the authors as an optimum. However, the acoustic field distribution was far from homogeneous. This situation provides an opportunity to optimize the acoustic field distribution.

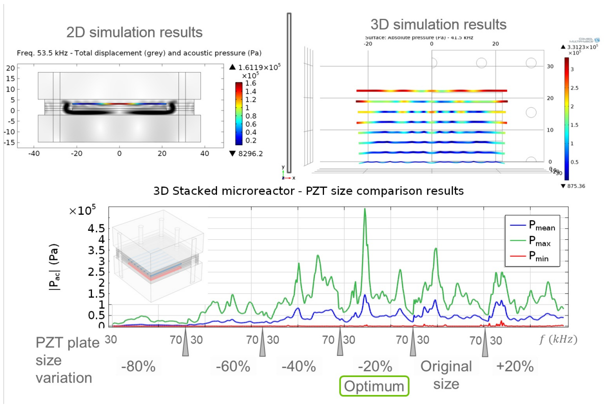

Figure 4: A frequency sweep (30-70 kHz) for each size of the PZT plate shows how, by reducing its size by 20%, the acoustic pressure obtained increases within the microchannels in a stacked-type sono-microreactor. Consequently, PZT material and energy consumption can be reduced