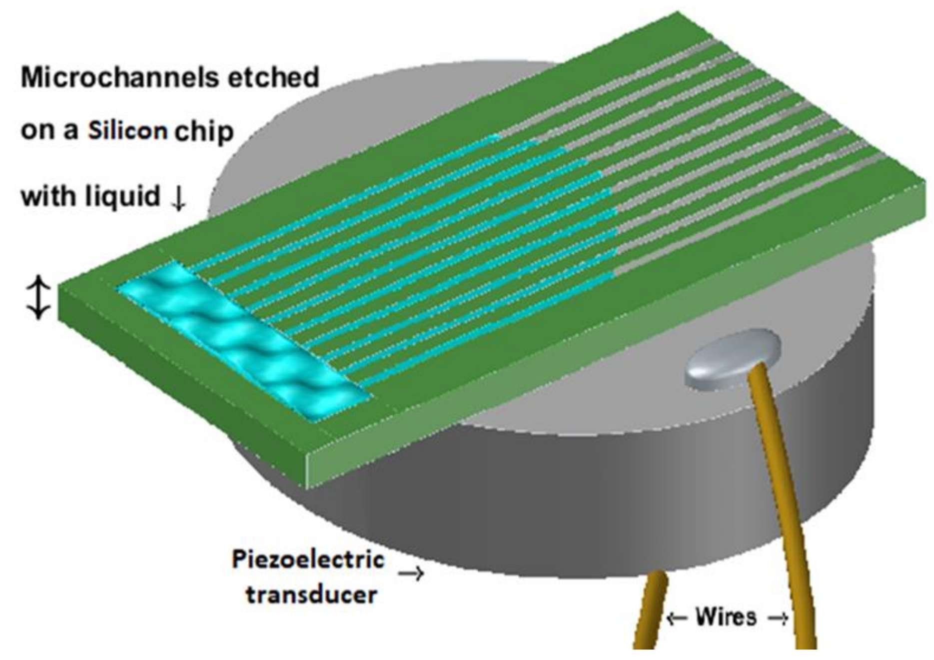
A Computational Study of Aerosol Droplet Formation for Personalised Airway and Lung Management (PALM)

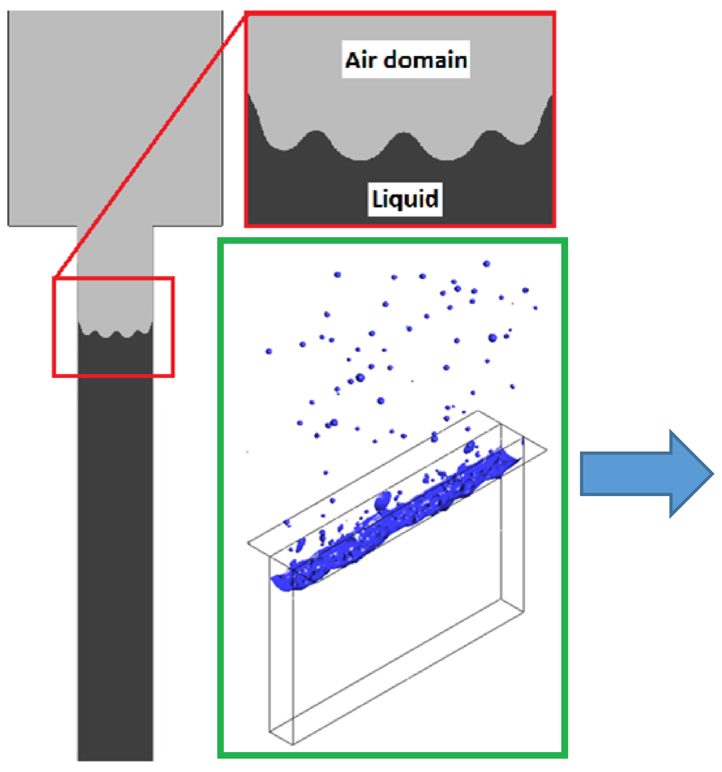
Abanoub Shenoda, Jason Brenker, Jackson Gum & Tuncay Alan

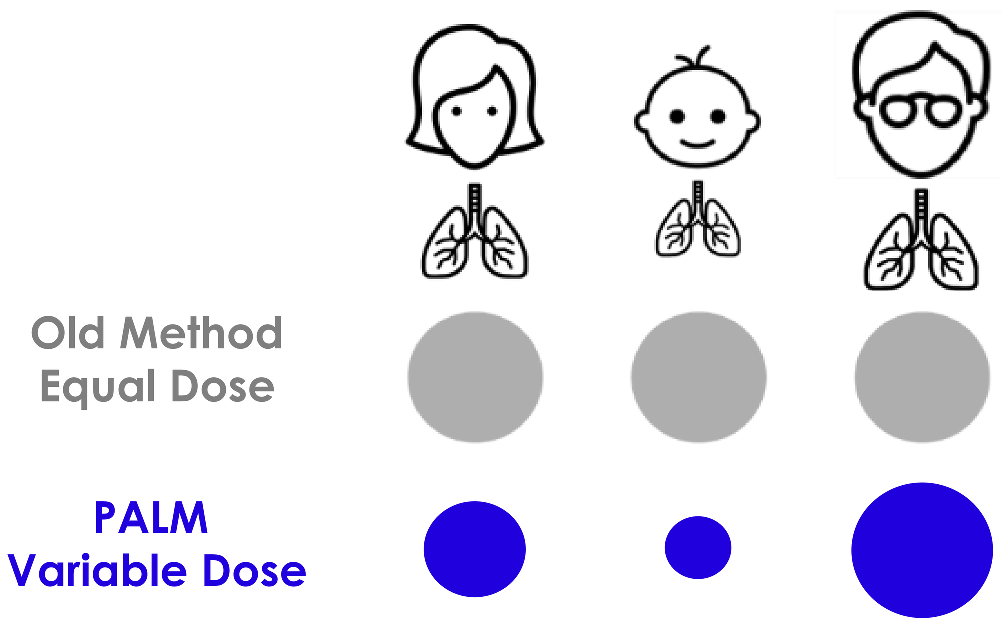
Monash University, Department of Mechanical and Aerospace Engineering, Melbourne VIC, 3800 Australia

Abanoub.Shenoda@monash.edu, Jason.Brenker@monash.edu, Jackson.Gum@monash.edu & Tuncay.Alan@monash.edu

Patented microfluidic technology







Unique sample delivery

Capillary filling of the liquid sample to be confined inside hydrophilic microchannels

Well defined interface & controlled wavelengths

The wavelength of the capillary waves is tuned by dialing the frequency

Tunable droplets

Breath actuated aerosol generation

Interface stability and aerosol formation

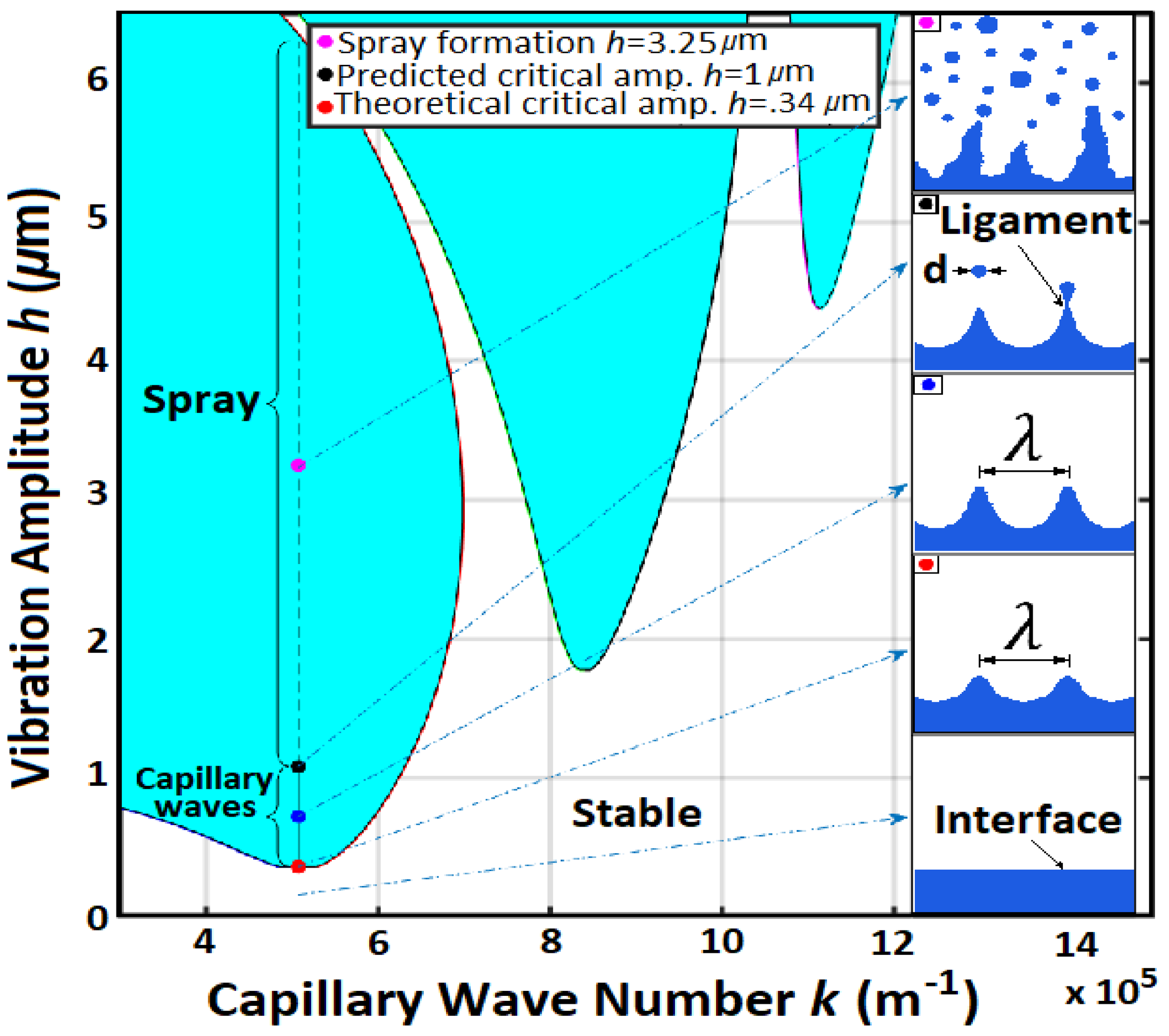


Figure 1: The damped Mathieu stability chart for liquid water actuated at 1 MHz. Cyan (unstable), white (stable), and the minimum (red) point indicates the theoretical critical threshold (0.34 μm) for droplet ejection. Insets are schematic representations of the spray formation stages starting from a flat interface followed by generation of capillary waves.

- **The damped Mathieu equation (Eq.1) [1] is used to examine interface stability:**

$$\ddot{H}(T) + 2\mu\dot{H}(T) + (p + 2q\cos(2T))H(T) = 0 \qquad (1)$$

H(T): is the unsteady capillary wave amplitude,

p: is a constant that depends on liquid properties and forcing frequency, and

q: is another constant that depends on liquid properties, forcing frequency, and vibration amplitude.

- **The theoretical critical amplitude after which the capillary waves break up into droplets is $a_c = 2(\mu/\rho)(\rho/\pi\sigma f)^{(1/3)}$ [2].**
- **The number median droplet diameter (Dn50) from ultrasonic nebulisers is predicted by Lang's experimental equation (Eq. 2) [3]. Accordingly,**

$$\mathrm{Dn50} = C\lambda = C(8\pi\sigma/\rho f^2)^{1/3} \qquad (2)$$

- **Lang's constant (C=0.34) does not always predict Dn50 accurately at MHz**

Numerical simulations

- **Spray formation requires a forcing amplitude greater than the predicted critical amplitude which is 1 μm at 1 MHz for water.**
- **The forcing frequency and critical amplitude are inversely proportional.**
- **Figure (2) shows a qualitative comparison of the capillary waves and ligaments formation which break up into main and satellite droplets at 1, 2.5, and 4 MHz.**
- **From (Fig. 3), as frequency increases, the mean droplet diameter decreases.**

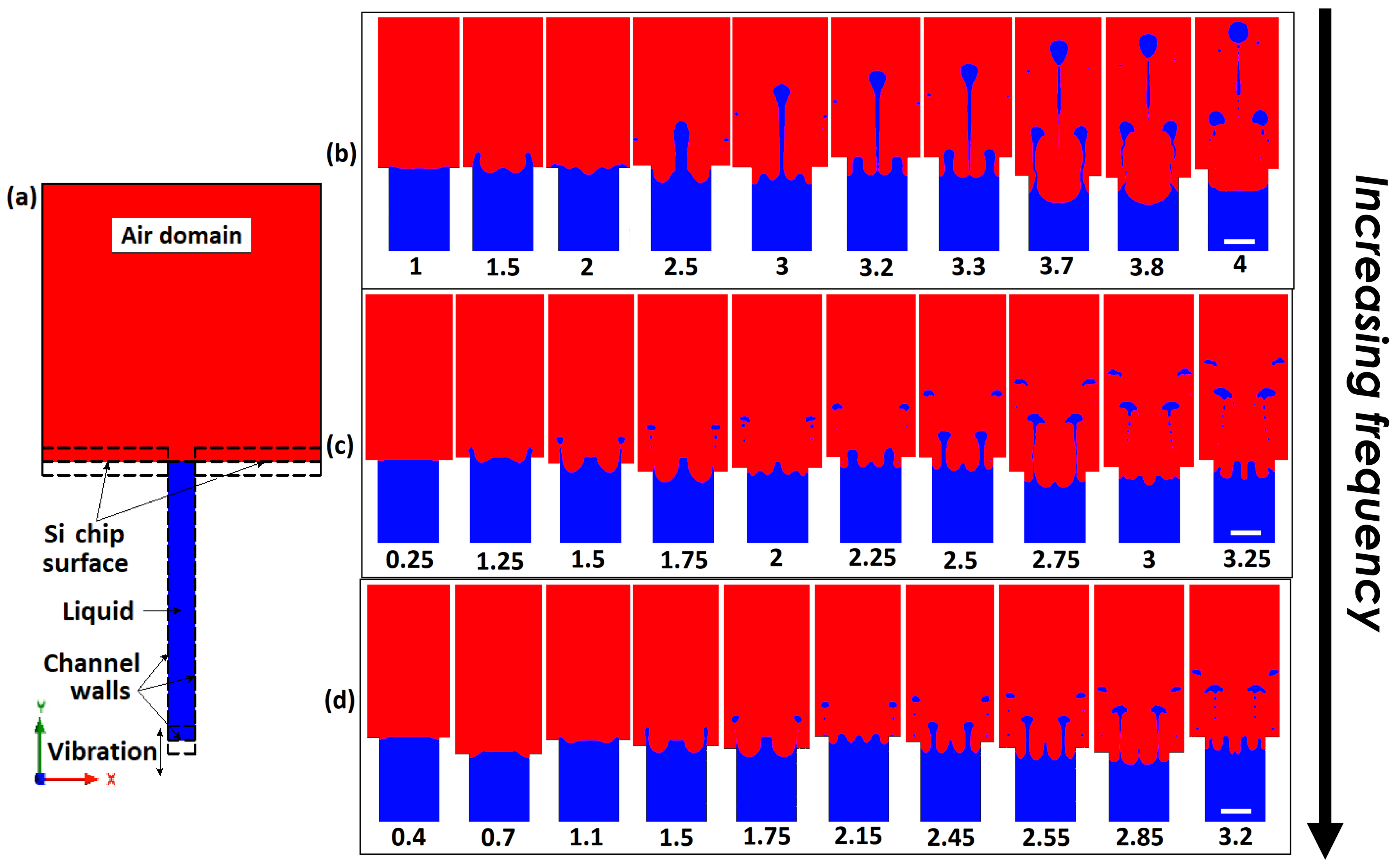


Figure 2: (a) CFD 2D model of the PALM and the dashed lines vibrate vertically. 2D CFD snapshots for ligament formation and their breakup into droplets being ejected from a microchannel filled with water vibrated at different forcing frequencies and amplitudes. At (b) 1 MHz & 3.25 μm, (c) 2.5 MHz & 2.5 μm, and (d) 4 MHz & 2 μm. The values beneath every simulation represent the number of cycles of vibrations. All white bars are 10 μm.

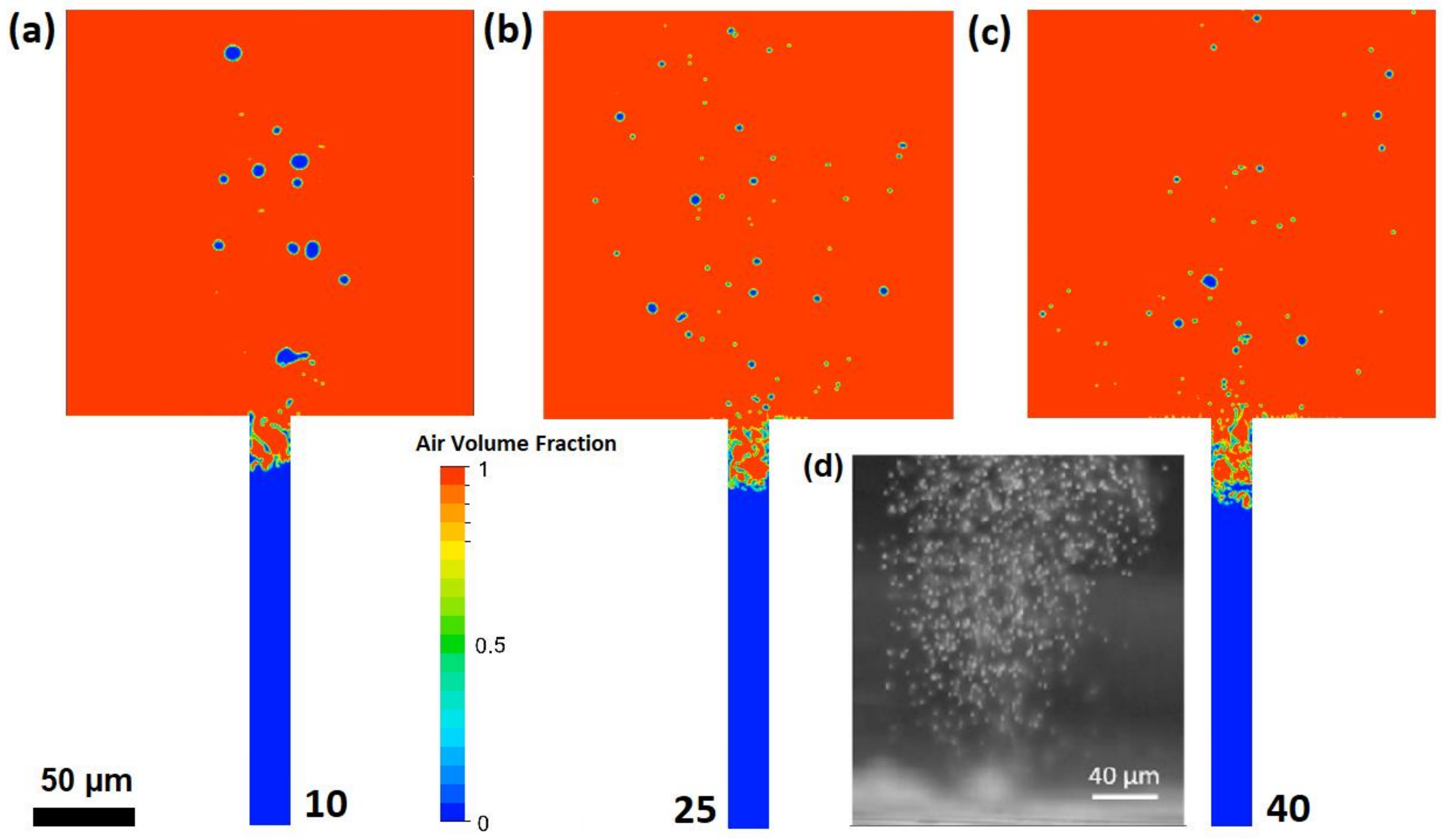


Figure 3: 2D CFD snapshots for spray formation at (a) 1 MHz & 3.25 μm, (b) 2.5 MHz & 2.5 μm, and (c) 4 MHz & 2 μm. (d) Snapshot of droplets as they leave the microfluidic chip. Recorded at 30,000 fps.

Conclusions

1) **The CFD simulations predict the droplet formation mechanism and bounding the liquid and controlling the wavelengths are necessary to tune droplet size.**
2) **Based on the CFD simulations, the onset of droplet ejection occurs at (1 μm) which is 3x the predicted value (0.34 μm) as expected (from 3 to 6) [3].**
3) **The higher the frequency the smaller the aerosol mean droplet diameter.**

References

1. Tsai S C et al., IEEE Trans Ultrason Ferroelectr Freq Control 2009, 56.9; pp 1968-1979.
2. Al-Suleimani Y et al., Proc. ILASS-Europe99 1999.
3. Lang R J, JASA 1962, 34.1: pp 6-8.

Drug Delivery to the Lungs (DDL), Edinburgh, UK, 7-9 12 2022