Supplementary Materials

For

Numerical Simulation and Investigation of System Parameters of Sonochemical Process

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In this section we have provided the entire graphical results of simulation for radial motion of cavitation bubble dynamics model. The graphical results present the effects of various parameters which are directly involved in sonochemical process. The parameters which were thoroughly investigated in this present work are: (1) Initial bubble size in the liquid medium, (2) Static pressure of the system, (3) System operating temperature, (4) Type of dissolved gas content and (5) Type of solvent or cavitation medium.

In section A.1 – A.5, the results show how the following parameters are changes with time scale during transient collapse of cavitation bubble. (A) radius of the bubble; (B) temperature inside the bubble; (C) water vapor evaporation in the bubble; (D) pressure inside the bubble; (E) micro–turbulence generated by the bubble; (F) acoustic waves emitted by the bubble. The effects of initial bubble radius are presented in Figs. S.1 – S.5, while Figs. S.6 – S.10 represent the effects of static pressure in sonochemical reaction. As the temperature increases the sonochemical effects decreases significantly as shown in Figs. S.11 – S.15. The dissolved also plays an important role in production of oxidizing species during transient collapse of cavitation bubbles. The simulation results for different gas bubbles dissolved in water are given in Figs. S.16 – S.19, and the trend of production of $^{\bullet}$OH radical per bubble with various dissolved gas bubbles is as follows: O_2 > Air > Ar > N_2. The simulation results of radial motion of cavitation bubble for various solvents with different physicochemical properties are shown in Figs. S.20 – S.21. This can be attributed to the lower surface tension and higher vapor pressure of the organic solvent. The production of $^{\bullet}$OH radical in water is always higher than that of in toluene and n-hexane. So, due to the low intensity of bubble collapse, organic solvents are not able to generate sufficient numbers of radical *in–situ* for sonochemical reactions.

Section A.1:

Simulations of radial motion with different initial air bubble radius in water. f = 20 kHz; P_A= 150 kPa; P_o= 100 kPa. Time history of (A) radius of the bubble; (B) temperature inside the bubble; (C) water vapor evaporation in the bubble; (D) pressure inside the bubble; (E) micro–turbulence generated by the bubble; (F) acoustic waves emitted by the bubble.

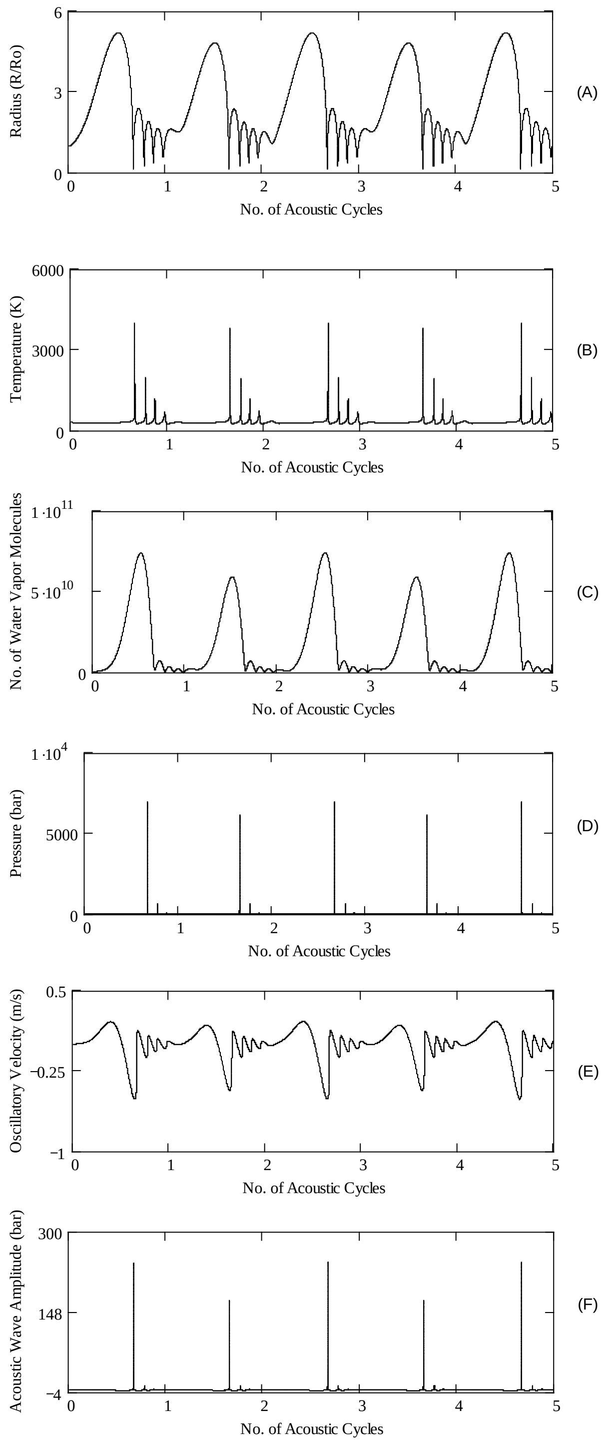

Figure S.1: 5 micron air bubble

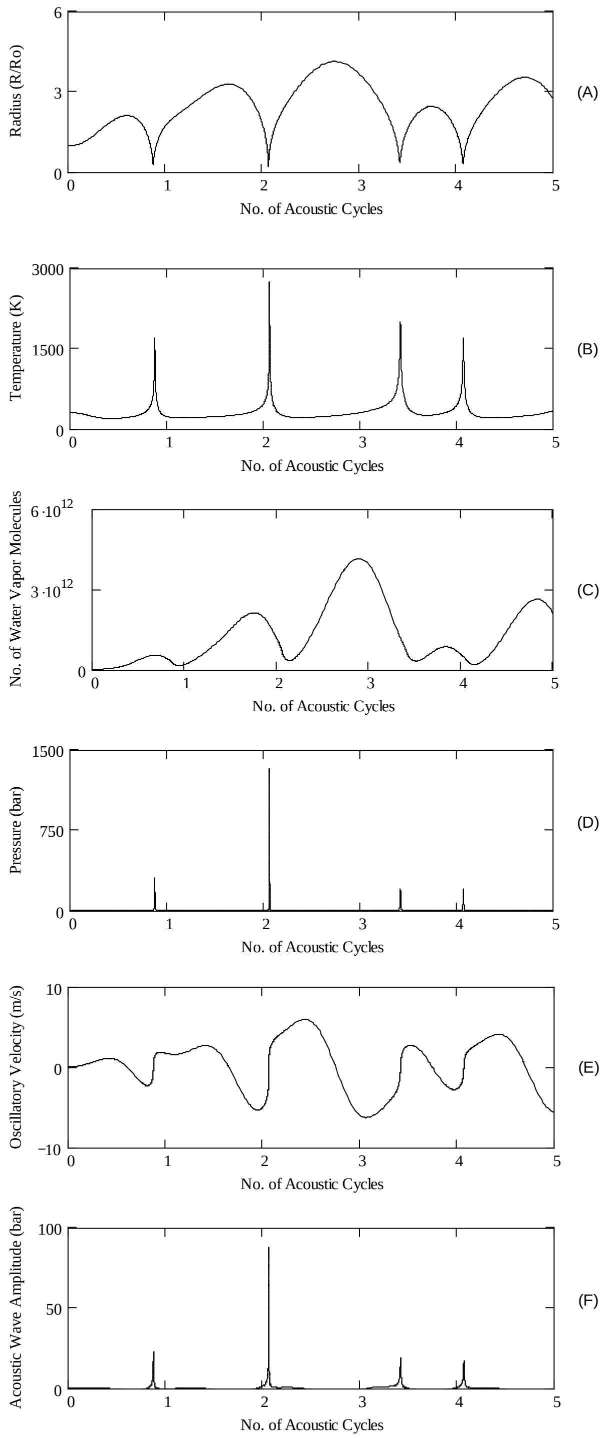

Figure S.2: 25 micron air bubble

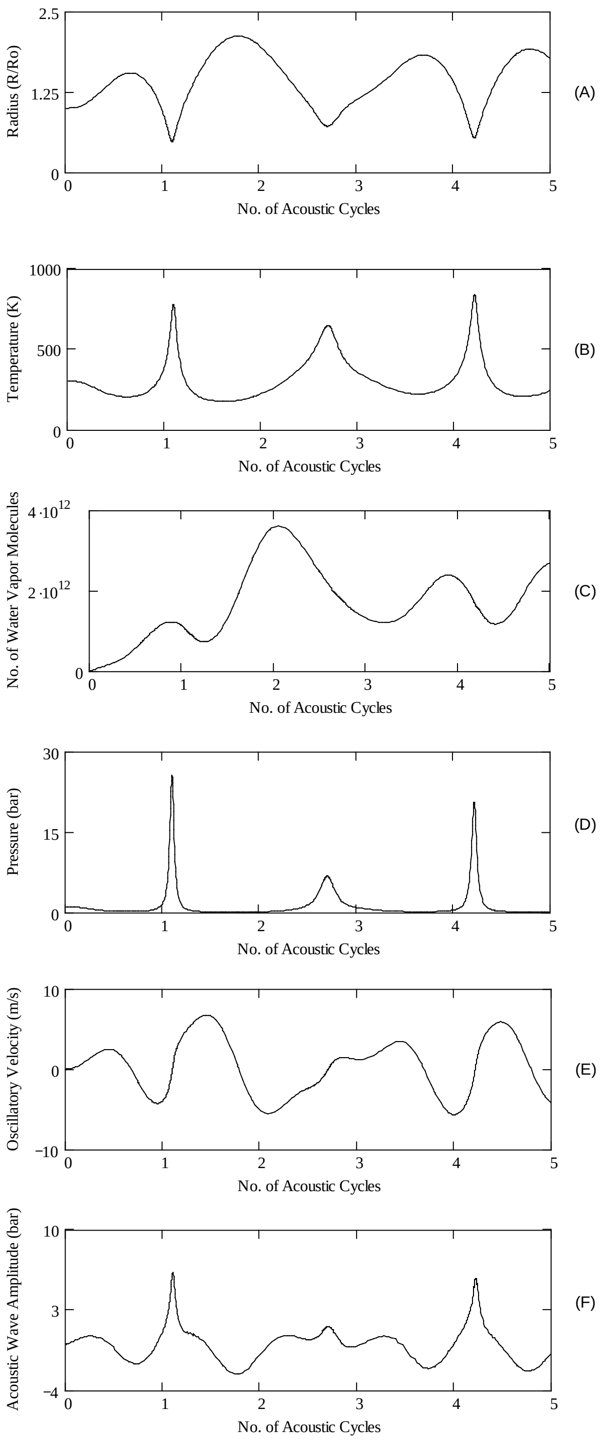

Figure S.3: 50 micron air bubble

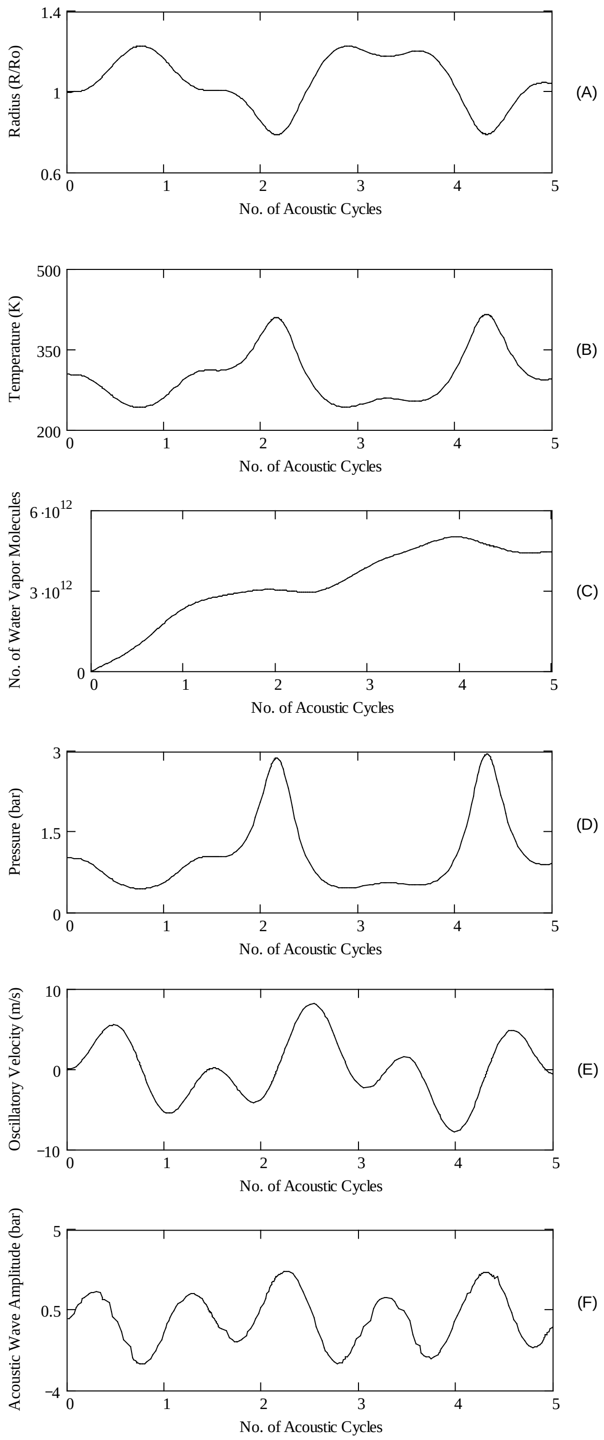

Figure S.4: 100 micron air bubble

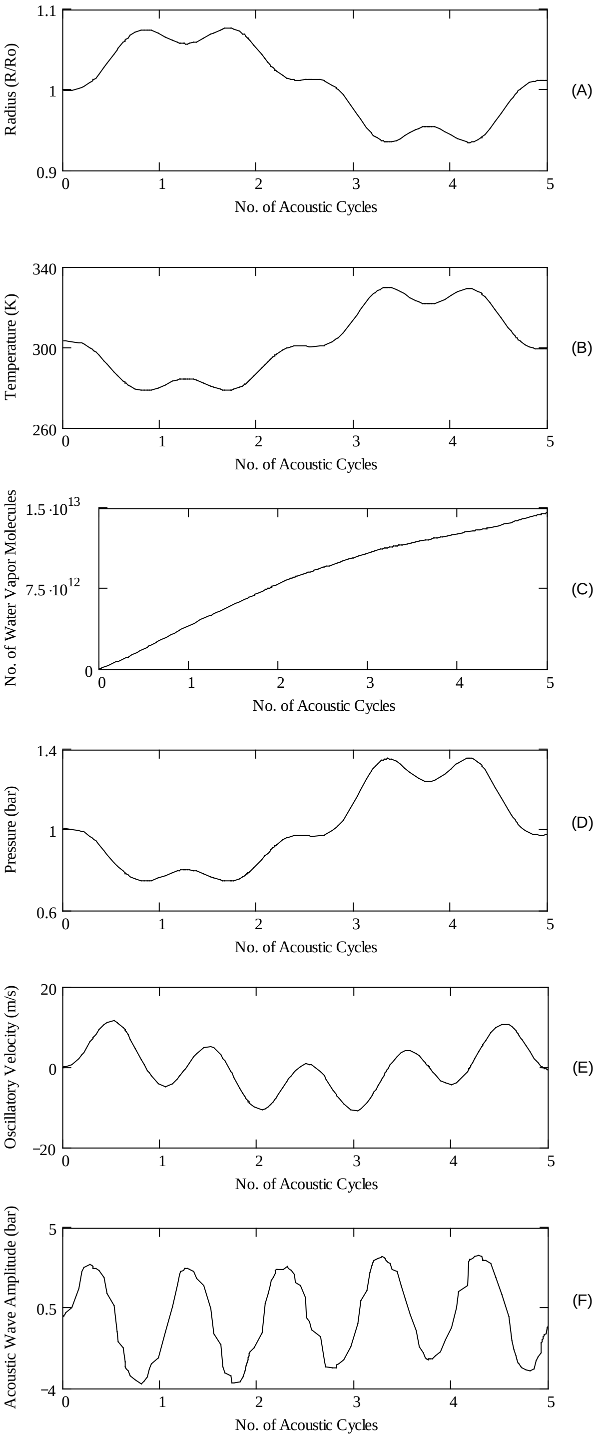

Figure S.5: 200 micron air bubble

Section A.2:

Simulations of radial motion of 5 micron air bubble in water under various static pressures. f = 20 kHz; P_A= 150 kPa; R_o= 5 µm. Time history of (A) radius of the bubble; (B) temperature inside the bubble; (C) water vapor evaporation in the bubble; (D) pressure inside the bubble; (E) micro–turbulence generated by the bubble; (F) acoustic waves emitted by the bubble

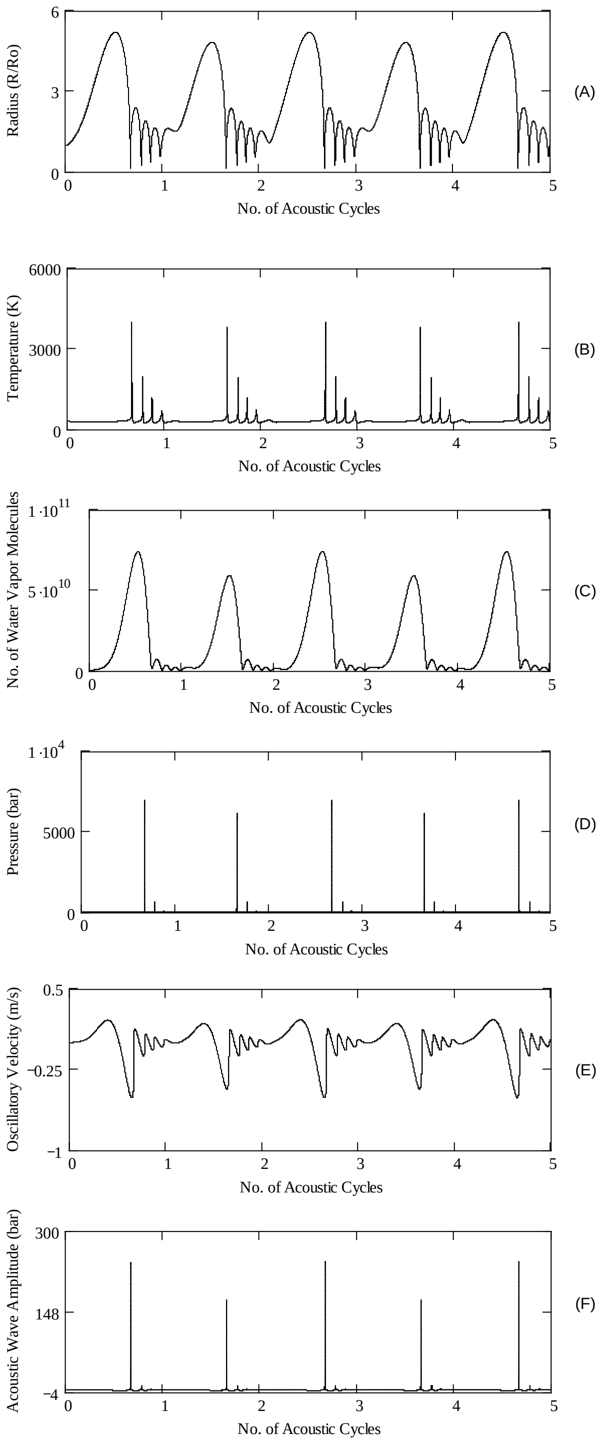

Figure S.6: 100 kPa

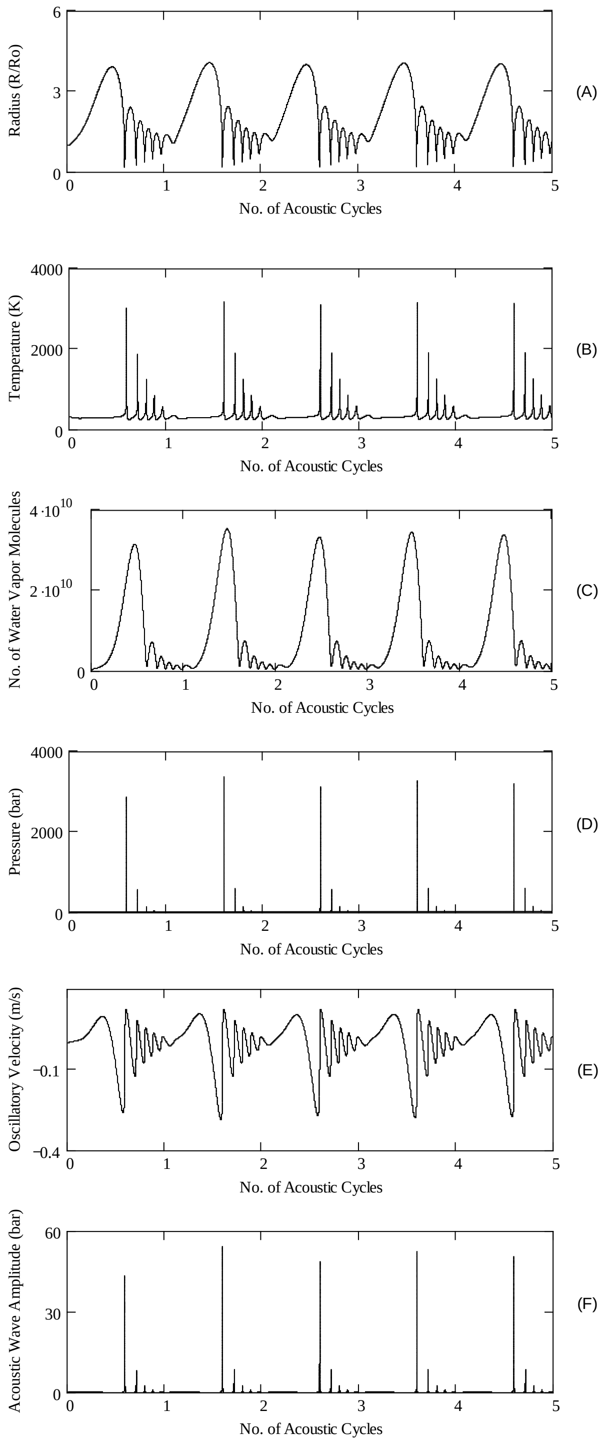

Figure S.7: 120 kPa

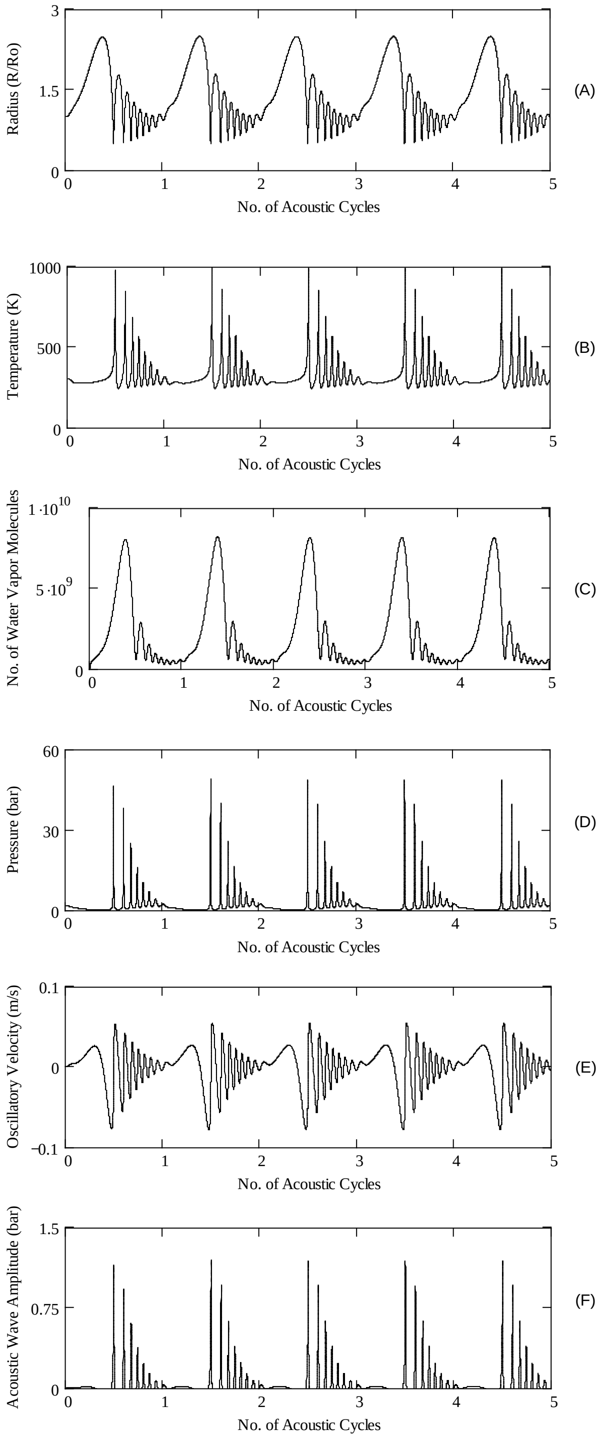

Figure S.8: 150 kPa

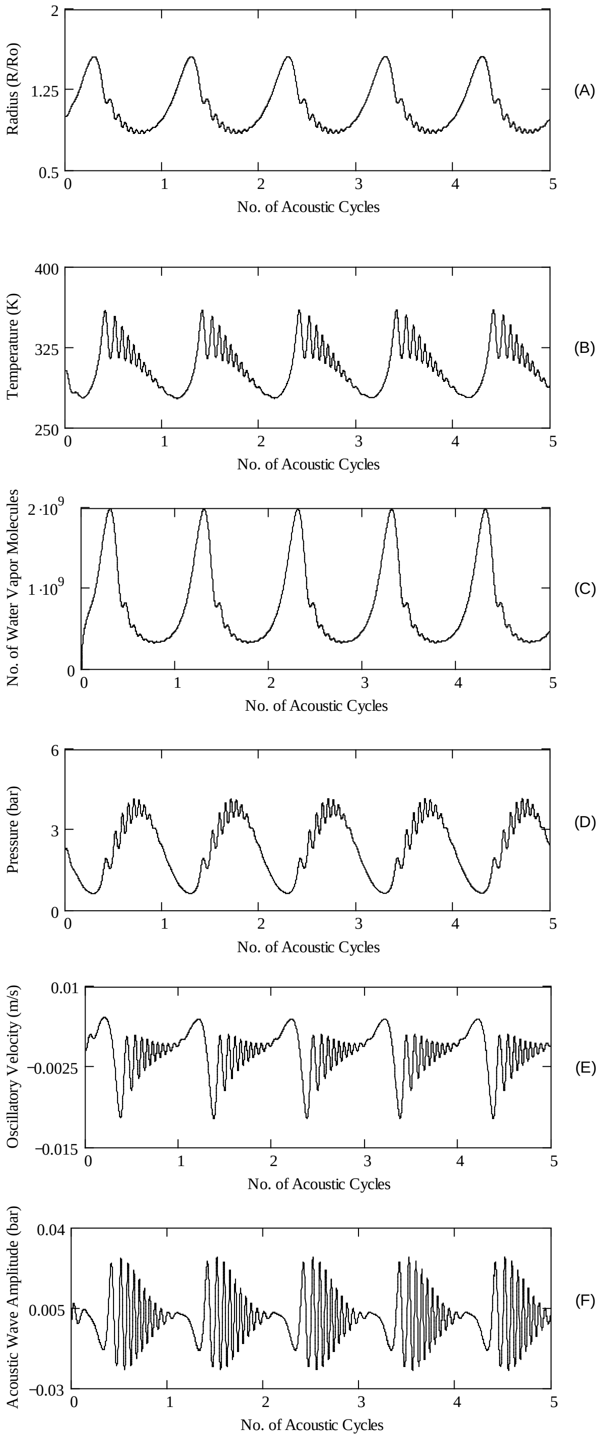

Figure S.9: 200 kPa

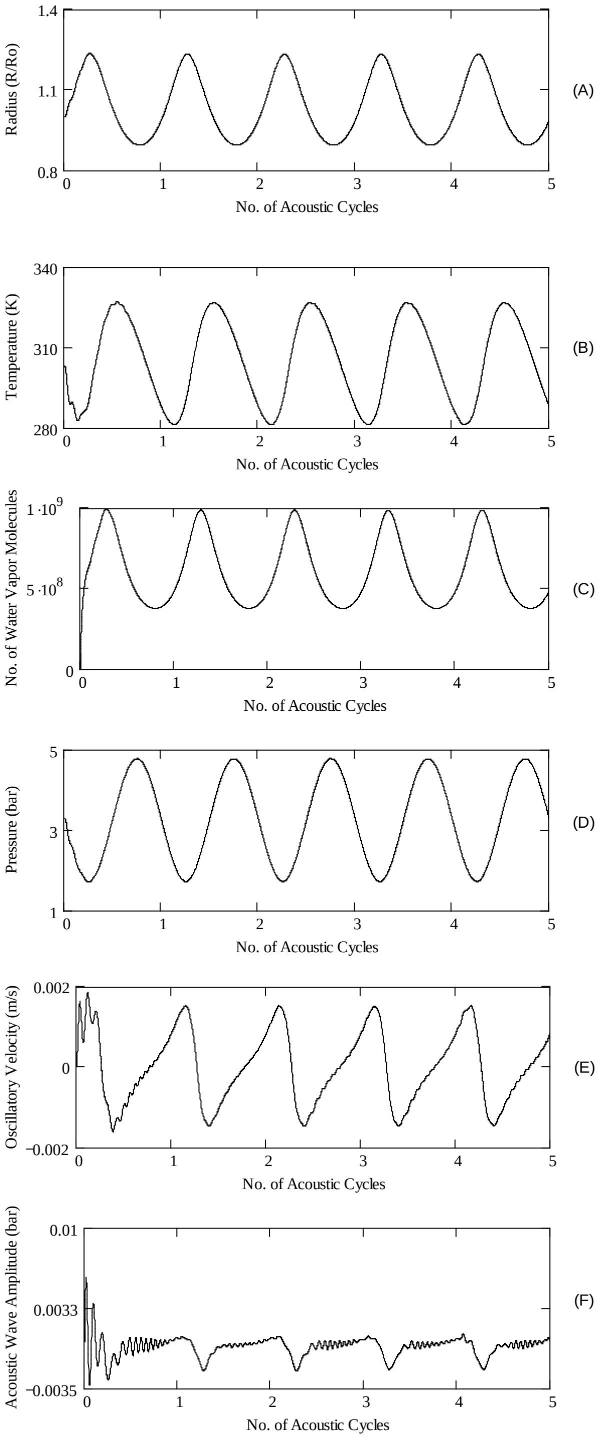

Figure S.10: 300 kPa

Section A.3:

Simulations of radial motion of 5 micron air bubble in water at different temperatures. f = 20 kHz; P_A= 150 kPa; P_o= 100 kPa. Time history of (A) radius of the bubble; (B) temperature inside the bubble; (C) water vapor evaporation in the bubble; (D) pressure inside the bubble; (E) micro–turbulence generated by the bubble; (F) acoustic waves emitted by the bubble

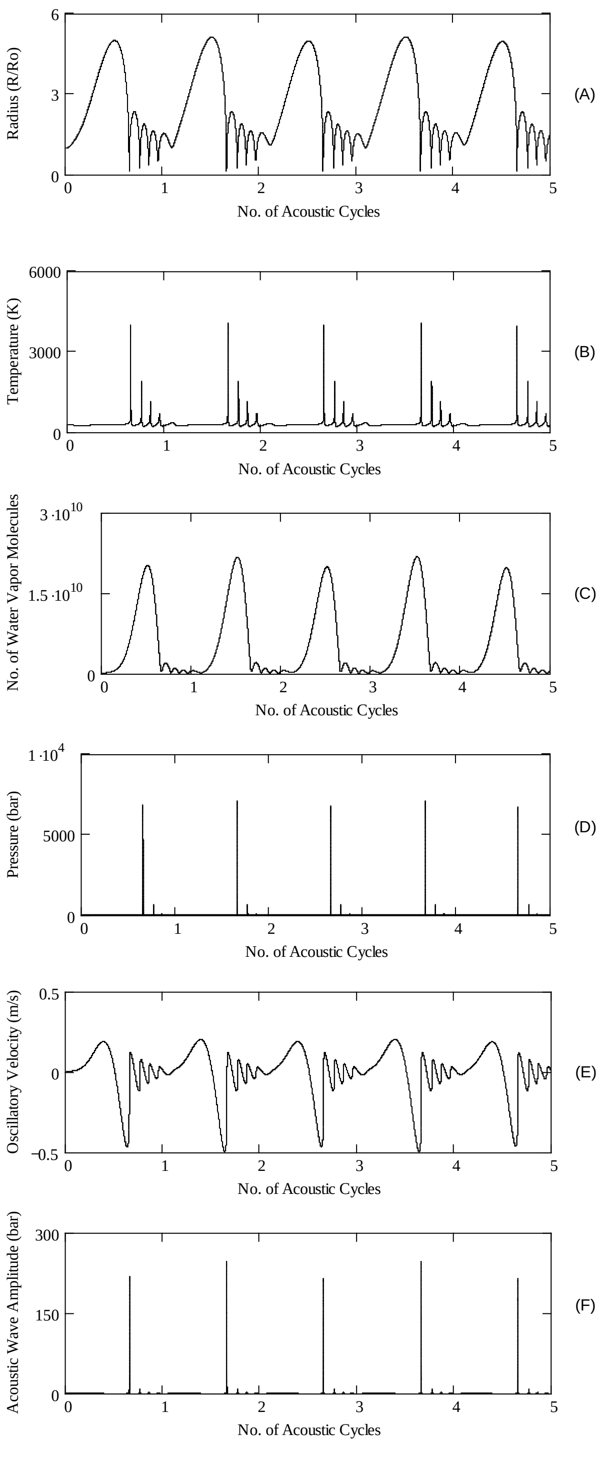

Figure S.11: 283 K

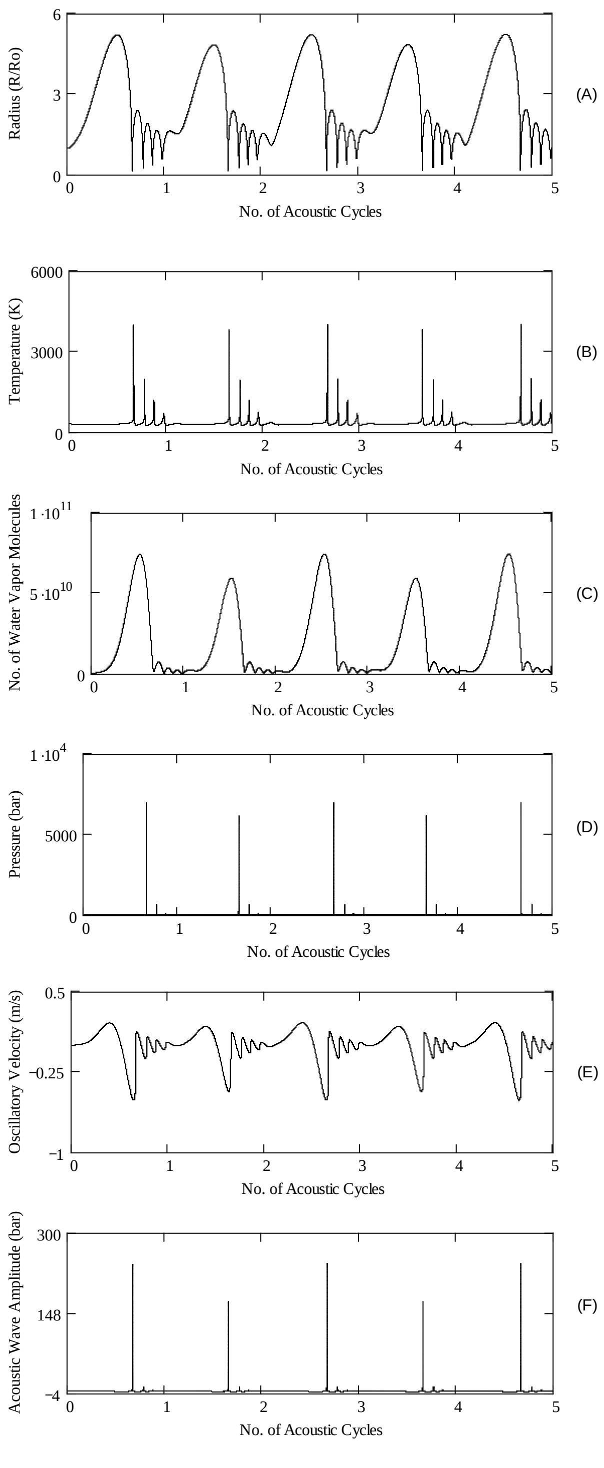

Figure S.12: 303 K

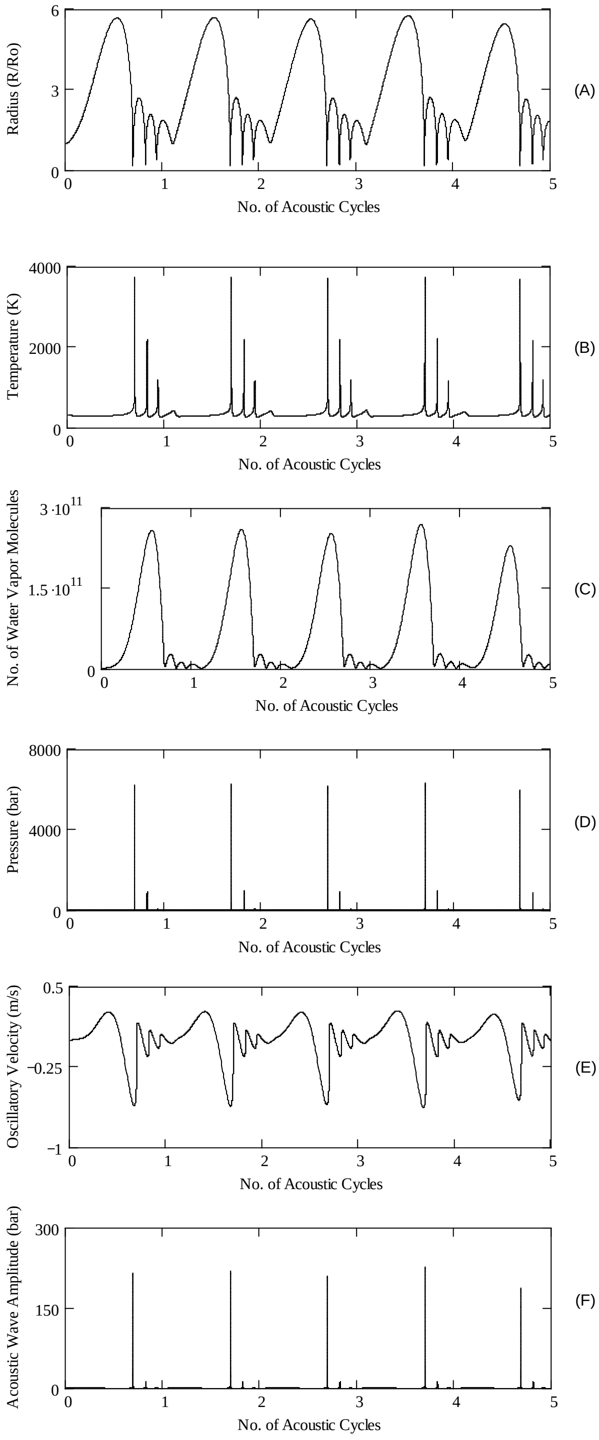

Figure S.13: 323 K

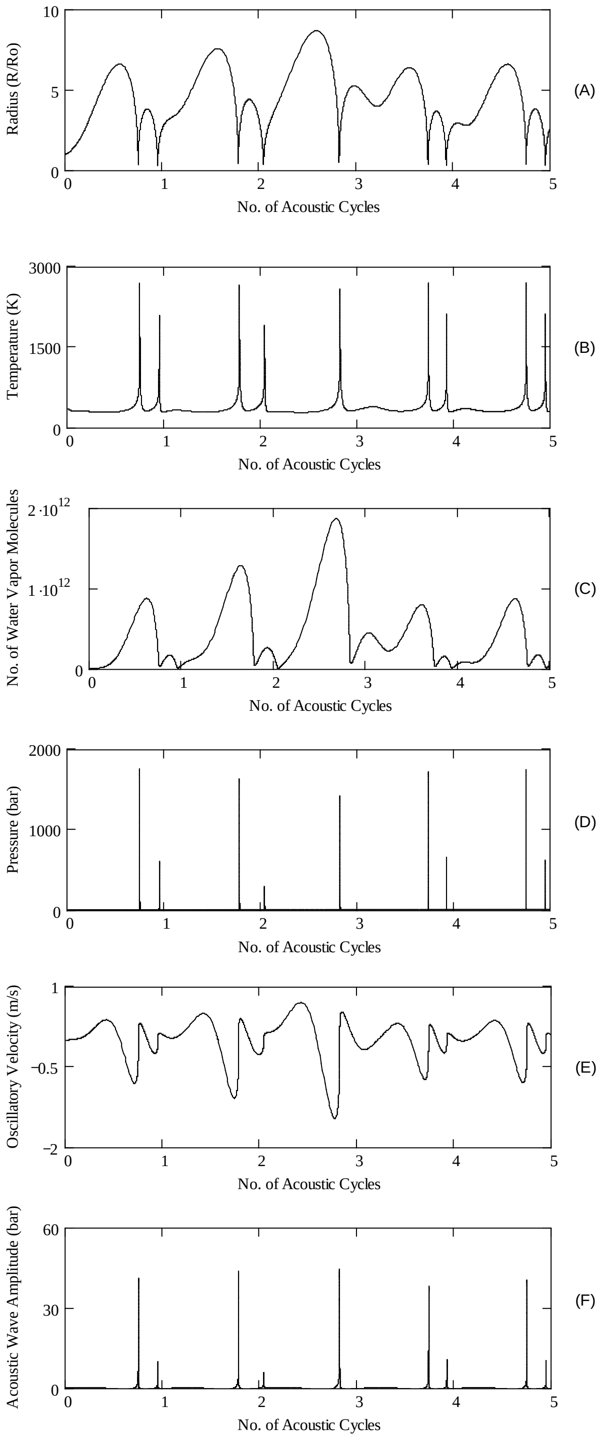

Figure S.14: 343 K

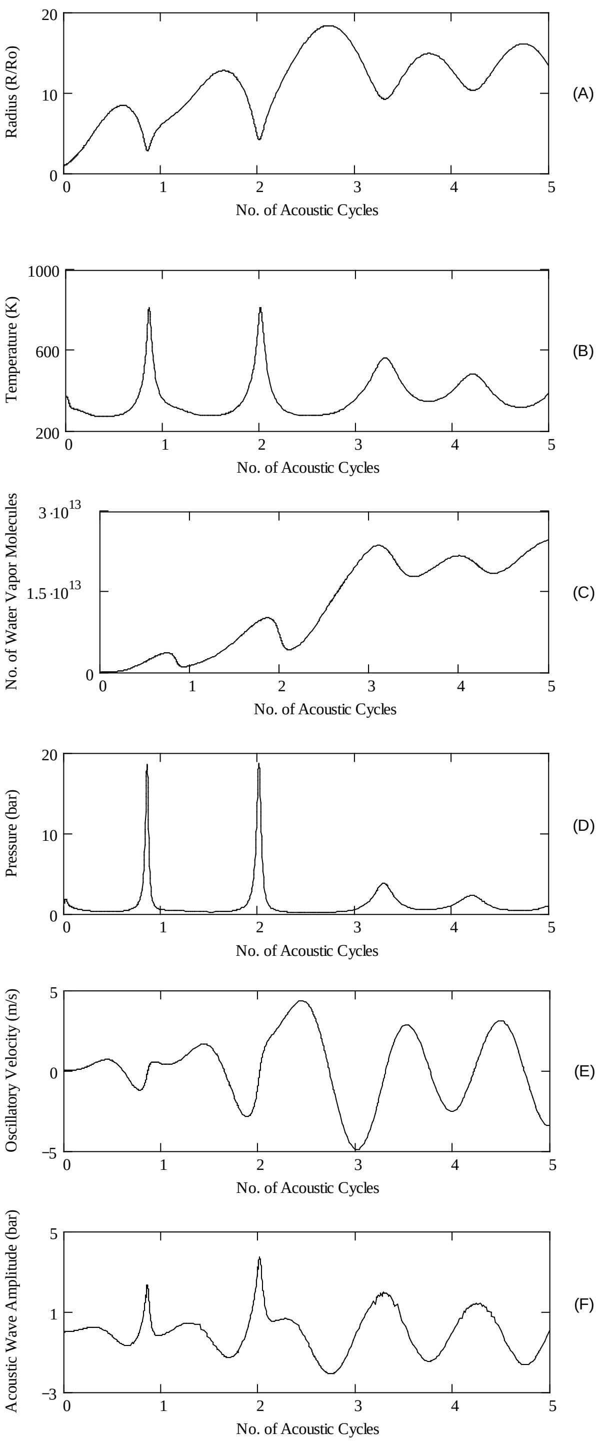

Figure S.15: 373 K

Section A.4:

Simulations of radial motion of 5 micron air bubble in water with different gas bubbles dissolved in water. f = 20 kHz; P_A= 150 kPa; P_o= 100 kPa. Time history of (A) radius of the bubble; (B) temperature inside the bubble; (C) water vapor evaporation in the bubble; (D) pressure inside the bubble; (E) micro–turbulence generated by the bubble; (F) acoustic waves emitted by the bubble.

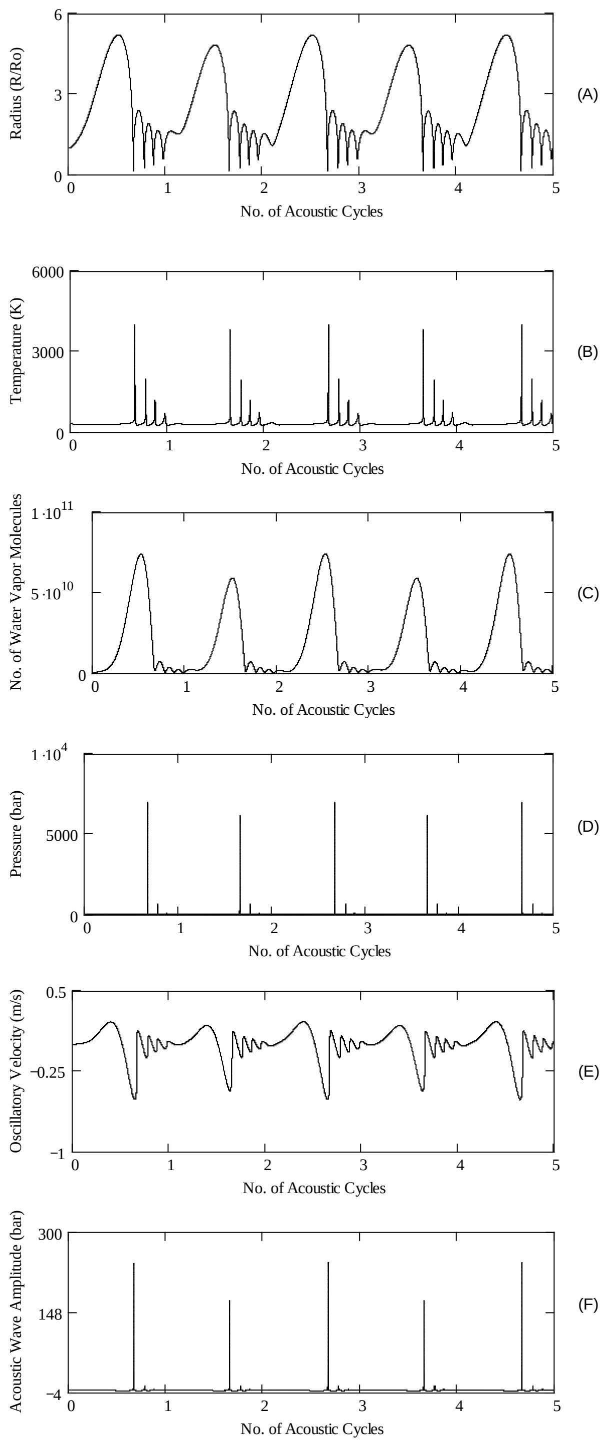

Figure S.16: Air bubble

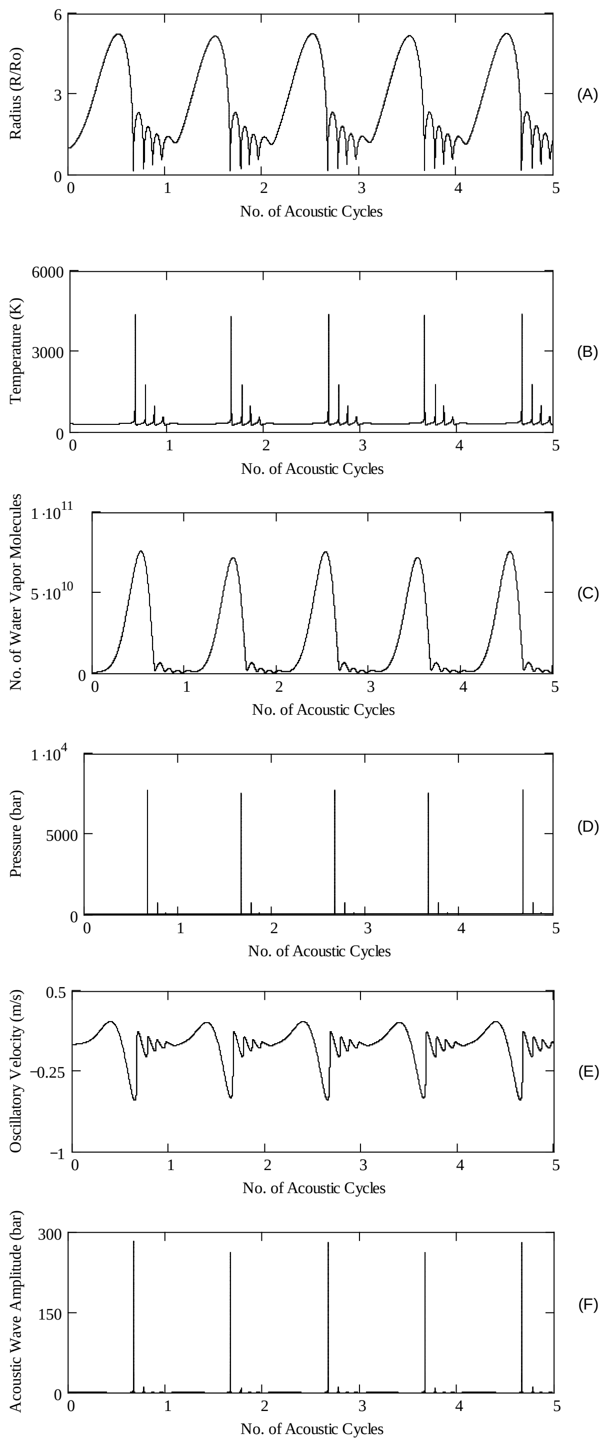

Figure S.17: Nitrogen bubble

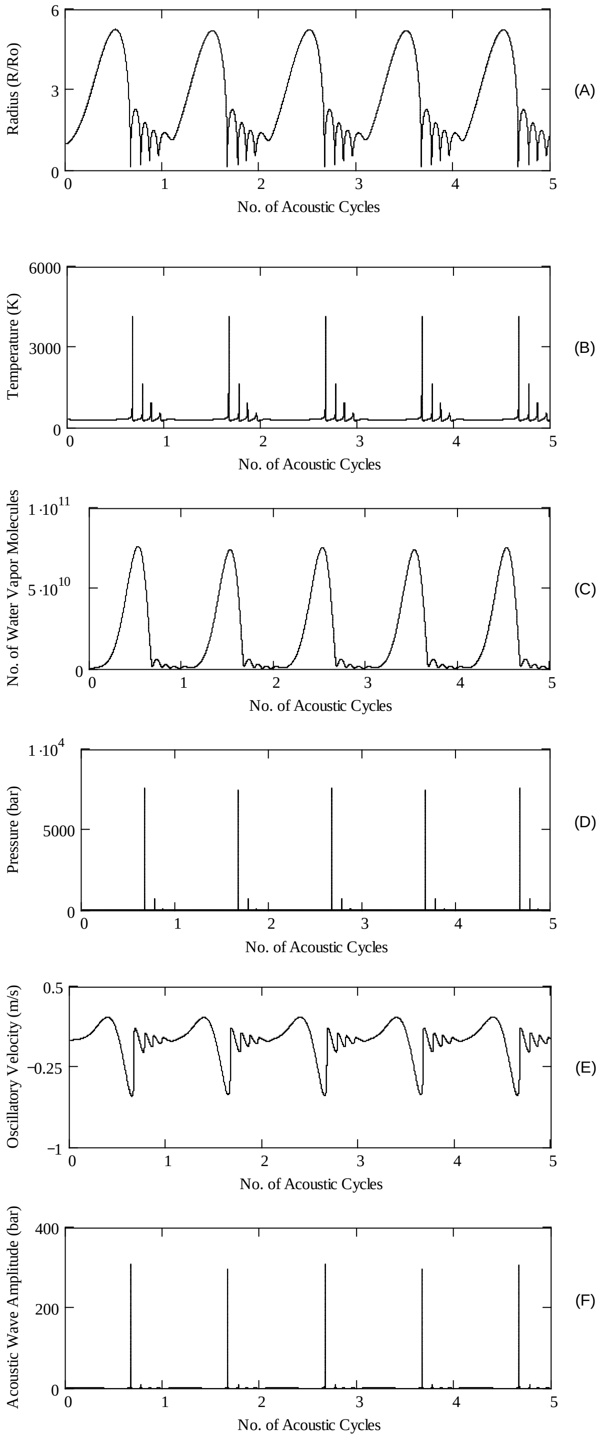

Figure S.18: Oxygen bubble

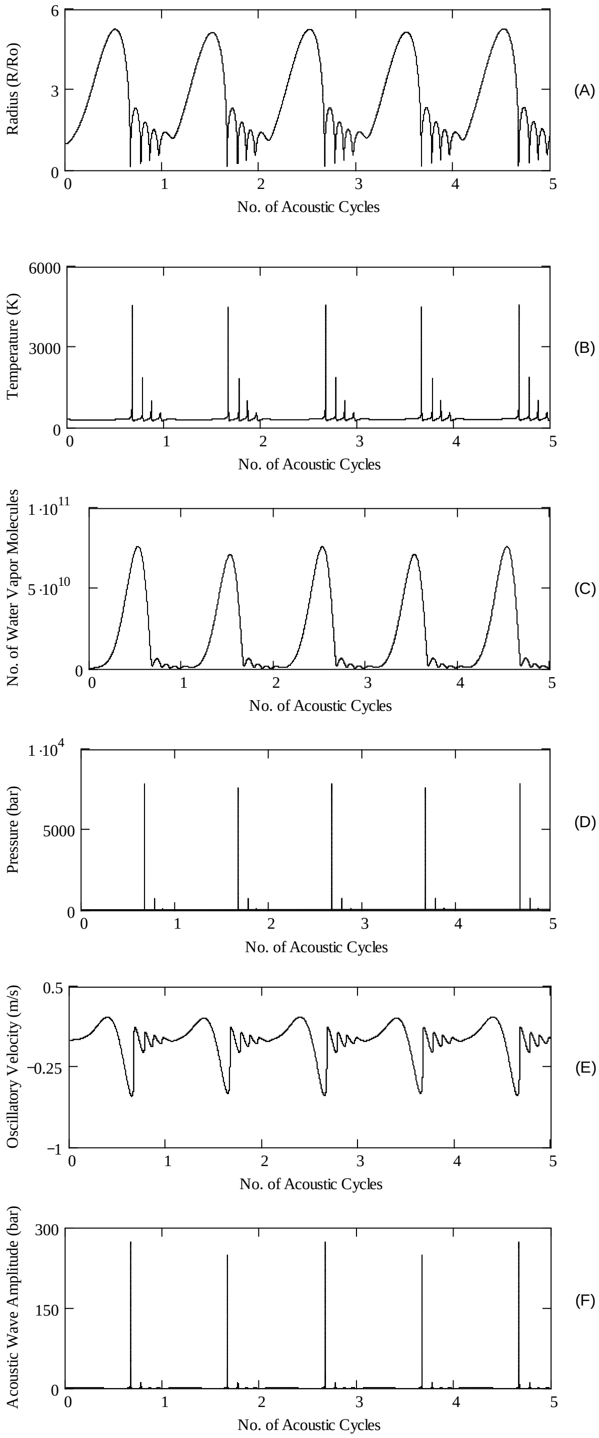

Figure S.19: Argon bubble

Section A.5:

Simulations of radial motion of 5 micron air bubble in toluene and n–hexane as cavitation medium. f = 35 kHz; P_A= 150 kPa; P_o= 100 kPa. Time history of (A) radius of the bubble; (B) temperature inside the bubble; (C) water vapor evaporation in the bubble; (D) pressure inside the bubble; (E) micro–turbulence generated by the bubble; (F) acoustic waves emitted by the bubble

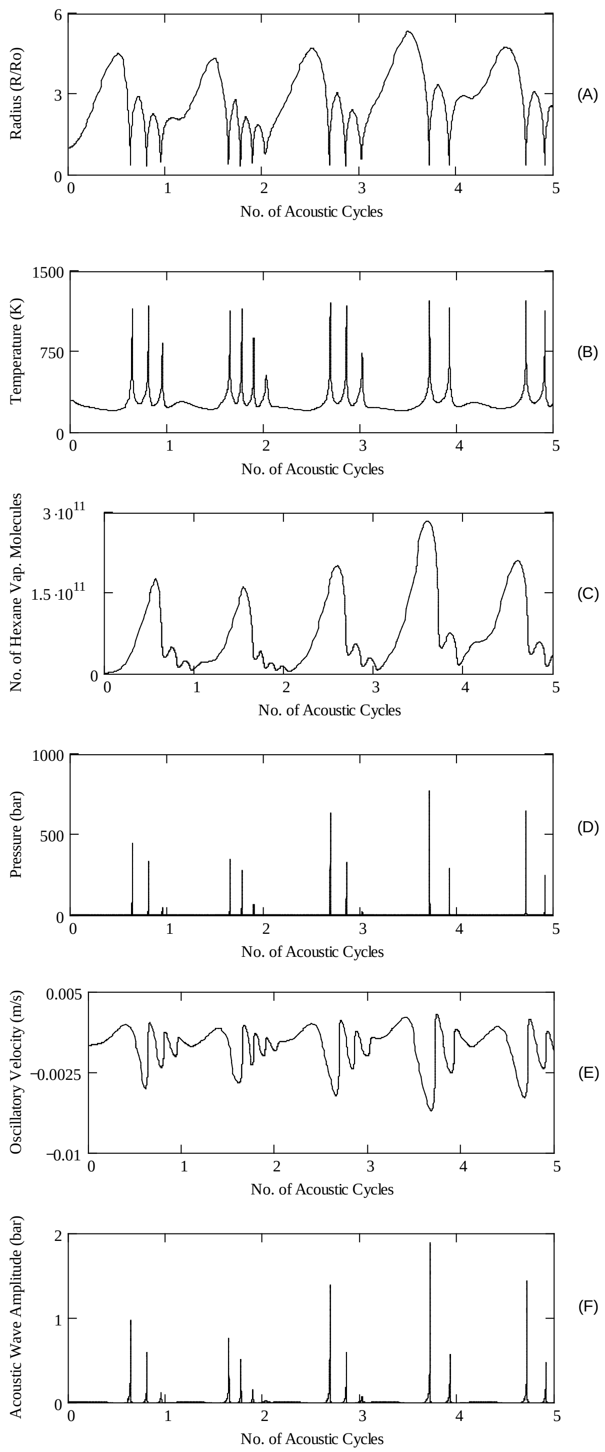

Figure S.20: n–Hexane

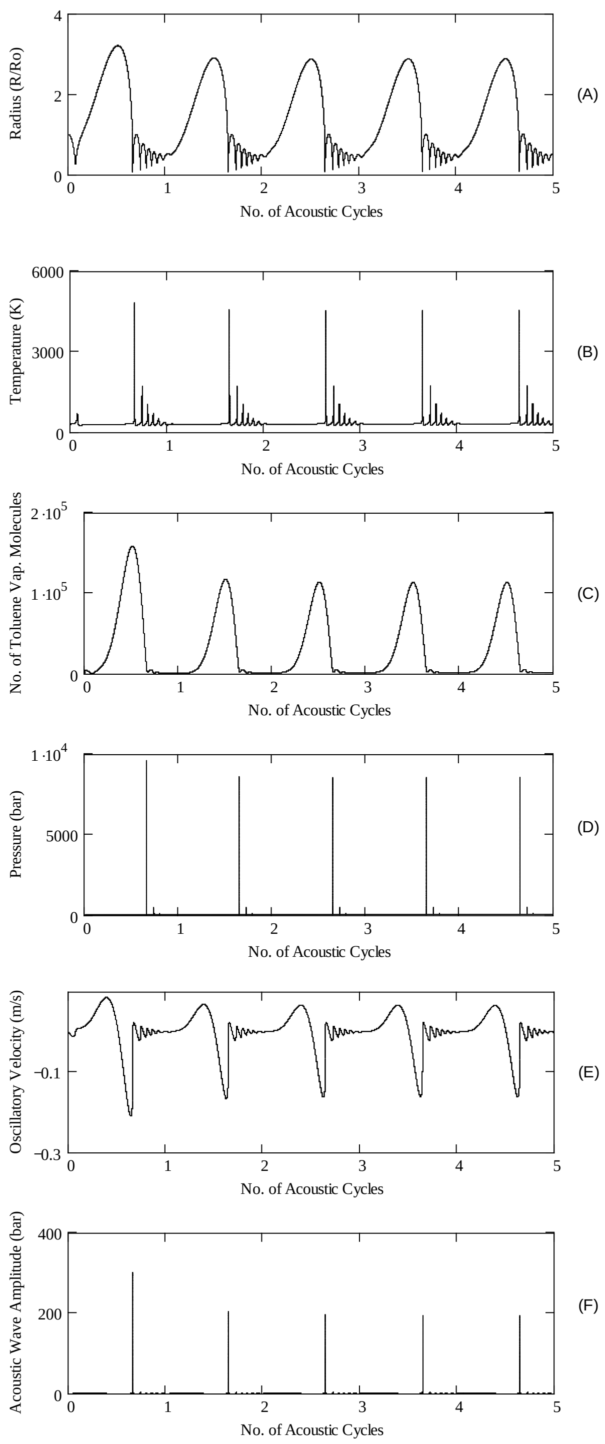

Figure S.21: Toluene