OPTIMAL BUBBLE TEMPERATURE FOR THE SONOCHMICAL PRODUCTION OF OXIDANTS IN WATER

K.Yasui[+], T.Tuziuti[+], and Y.Iida[+]

+National Institute of Advanced Industrial Science and Technology (AIST),
2266-98 Anagahora, Shimoshidami, Moriyama-ku, Nagoya 463-8560, JAPAN
k.yasui@aist.go.jp

Abstract

Computer simulations of bubble oscillations in liquid water irradiated with ultrasound are performed under various amplitudes of ultrasound and various ambient pressures. In the computer simulations, non-equilibrium evaporation and condensation of water vapor at the bubble wall and that of chemical reactions of gases and vapor inside a bubble are taken into account. The oxidants such as OH radicals, O radicals, H_2O_2 molecules, and O_3 molecules are created from water vapor inside a bubble when a bubble collapses violently and the temperature inside a bubble increases dramatically. The computer simulations have revealed that there exists the optimal bubble temperature, which is about 5,500 K, for the production of the oxidants inside an air bubble because at higher bubble temperature the oxidants are strongly consumed inside a bubble by oxidizing nitrogen. Inside an oxygen bubble, on the other hand, the amount of the oxidants created inside a bubble increases as the temperature inside a bubble increases because nitrogen is absent.

Introduction

When a liquid is irradiated by a strong ultrasound, many tiny gas bubbles appear, which is called acoustic cavitation[1]. The tiny bubbles repeat expansion and contraction according to the pressure oscillation of ultrasound[2]. The speed of the bubble collapse sometimes reaches the sound velocity of the liquid[3] and the temperature and pressure inside a bubble increases dramatically because the work done by the liquid to compress the bubble is converted to heat which does not escape from the bubble so much by thermal conduction due to the high speed of the collapse[3,4]. The temperature and pressure inside a bubble at the collapse sometimes reach 10,000 K and 10,000 atm, respectively[3,4]. As a result, water vapor inside a bubble is dissociated and oxidants such as OH radicals, O radicals, H_2O_2 molecules, and O_3 molecules are created inside a bubble[5]. The oxidants diffuse out of the bubble into the surrounding liquid and solutes such as pollutants are dissociated by them[6]. Chemical reactions induced by ultrasound is called sonochemical reactions[6].

In the present study, computer simulations are performed for bubble oscillations in water irradiated by ultrasound of various pressure amplitudes under various ambient pressures in order to study the correlation between the bubble temperature at the collapse and the amount of oxidants created inside a bubble. In the literature[7], it was believed that the amount of oxidants created inside a bubble increases as the bubble temperature at the collapse increases. The present study has revealed that there exists an optimum bubble temperature for air bubbles, which is about 5,500 K, for the sonochemical production of oxidants and that at higher bubble temperature the amount of the oxidants created inside a bubble decreases considerably.

Model

In the present model, a spherical bubble is oscillating according to the pressure oscillation of ultrasound with the pressure and temperature inside a bubble being spatially uniform except at the thermal boundary layer near the bubble wall[8]. In the present model, the effect of non-equilibrium evaporation and condensation of water vapor at the bubble wall, of chemical reactions of gases and vapor inside a bubble, of thermal conduction both inside and outside a bubble, and of the liquid compressibility are taken into account[3,5,8]. Details of the present model is described in Refs.[3,5,8].

In the present study, computer simulations are performed for an air bubble and an oxygen bubble. For an air bubble, 93 chemical reactions and their backward reactions are taken into account. The most important chemical reactions are listed in Ref.[5].

Results

Computer simulations of bubble oscillations are performed under the experimental conditions of Refs.[9,10] for various acoustic amplitudes and various ambient pressures. The experiment of Ref.[9] is for air bubbles and that of Ref.[10] is for oxygen bubbles.

(A) Air bubbles

At first, we will see the calculated results for air bubbles under the experimental condition of Ref.[9].
The frequency of ultrasound is 140 kHz and the liquid temperature is 20^{o}C[9]. The ambient pressure studied ranges from 0.29 atm to 1 atm[9](In the calculation,

the ambient pressure of 2 atm is also studied). The ambient bubble radius is assumed to be 5 μm in the present computer simulations because it is a typical value at ultrasonic frequency of 140 kHz[11]. The computer simulations have revealed that the amount of oxidants created inside a bubble, which is OH radicals, O radicals, H_2O_2 molecules and O_3 molecules, is correlated with the bubble temperature at the collapse and that there exists an optimum bubble temperature for the production of oxidants, which is about 5,500 K[5].

It should be noted here that as there exists an optimum bubble temperature for the production of the oxidants there exists a corresponding optimum acoustic amplitude as described in detail in Ref.[5].

(B) Oxygen bubbles

Now we will see the calculated results for an oxygen bubble under the experimental condition of Ref.[10]. The frequency of ultrasound is 1 MHz and the liquid temperature is 20^{o}C[10]. The ambient bubble radius is assumed to be 0.5 μm in the present computer simulations because it is a typical value at ultrasonic frequency of 1 MHz[11,12]. The ambient pressure studied ranges from 1 atm to 3 atm[10].

Calculated results show that for an oxygen bubble the amount of the oxidants created inside a bubble increases as the bubble temperature at the collapse increases because nitrogen is absent and the oxidants are not consumed much inside a bubble[5].

Conclusion

Computer simulations of bubble oscillations under various acoustic amplitudes and various ambient pressures have revealed that there exists an optimum bubble temperature for the production of oxidants such as OH radicals, O radicals, H_2O_2 molecules, and O_3 molecules from water vapor inside an air bubble at the collapse because at higher bubble temeparture the oxidants are strongly consumed by oxidizing nitrogen. Correspondingly, there exists an optimum acoustic amplitude. For an oxygen bubble, on the other hand, the amount of the oxidants created inside a bubble increases as the bubble temperature at the collapse increases because nitrogen is absent and the oxidants are not consumed much inside a bubble.

Acknowledgements

This study was supported by Industrial Technology Research Grant Program in 2002 and 2003 from New Energy and Industrial Technology Development Organization (NEDO) of Japan.

References

[1] T.G.Leighton, The Acoustic Bubble, Academic Press, London, 1994.

[2] W.Lauterborn, T.Kurz, R.Mettin, C.D.Ohl, “Experimental and theoretical bubble dynamics,” Adv.Chem.Phys. vol. 110, pp.295-380, 1999.

[3] K.Yasui, “Effect of liquid temperature on sonoluminescence,” Phys.Rev.E, vol. 64, 016310, 2001.

[4] K.Yasui, “Temperature in multibubble sonoluminescence,” J.Chem.Phys., vol. 115, pp.2893-2896, 2001.

[5] K.Yasui, T.Tuziuti, Y.Iida, and H.Mitome, “Theoretical study of the ambient-pressure dependence of sonochemical reactions,” J.Chem.Phys. vol. 119, pp. 346-356, 2003.

[6] T.J.Mason(Ed.), Advances in Sonochemistry, Vols.1-6, JAI,London,1990-2001.

[7] T.Kondo, J.Gamson, J.B.Mitchell, P.Riesz, “Free-radical formation and cell-lysis induced by ultrasound in the presence of different rare-gases,” Int.J.Radiat.Biol., vol.54, pp.955-962, 1988.

[8] K.Yasui, “Alternative model of single-bubble sonoluminescence,” Phys.Rev.E , vol.56, pp.6750-6760,1997.

[9] T.Tuziuti, S.Hatanaka, K.Yasui, T.Kozuka, and H.Mitome, “Effect of ambient-pressure reduction on multibubble sonochemiluminescence,” J.Chem.Phys. vol.116, pp. 6221-6227, 2002.

[10] A.Henglein and M.Gutierrez, “sonochemistry and sonoluminescence – effect of external-pressure,” J.Phys.Chem., vol. 97, pp.158-162, 1993.

[11] K.Yasui, “Influence of ultrasonic frequency on multibubble sonoluminescence,” J.Acoust.Soc.Am. vol. 112, pp.1405-1413, 2002.

[12] K.R.Weninger, C.G.Camara, and S.J.Putterman, “Observation of bubble dynamics within luminescent cavitation clouds: sonoluminescence at the nano-scale,” Phys.Rev.E, vol. 63, 016310, 2001.