Modeling of ultrasonic cavitation as an advanced technique for water treatment

Slimane Merouani, Oualid Hamdaoui, Yacine Rezgui, Miloud Guemini

ABSTRACT

This paper presents a theoretical study of ultrasonic cavitation as an advanced technique for water treatment. A mathematical algorithm, which combines single bubble dynamics model with chemical kinetics mechanism for cavitating bubble, is proposed for estimating the chemical activity of cavitation bubbles. The computer simulations of bubble oscillation and chemical reactions occurring inside a bubble have been performed for various conditions of ultrasonic frequency. The numerical simulations have showed that radicals such as \( \cdot \text{OH}, \cdot \text{H}, \) and \( \cdot \text{O} \) are created in the bubble during the strong collapse. In all cases, \( \cdot \text{OH} \) is the main oxidant created in the bubble. It was found that the generation of the oxidants inside a bubble is strongly frequency dependent. The production rate of the oxidants decreased as the driving ultrasonic frequency increased. It was found that the reaction time is one of the paramount parameters of cavitation that control the extent of radical’s generation. Though a direct quantitative comparison between the predicted results in a single bubble and those in bulk solution is impossible, the present theoretical model is able to predict and explain the qualitative trend observed in some experimentally sonochemical phenomena.

Keywords: Ultrasonic cavitation; Bubble dynamics; Chemical Kinetics; Computer simulations; \( \cdot \text{OH} \) radicals