Scale-up Design of Ultrasound Irradiator for Advanced Oxidation Process (AOP) Using COMSOL Multiphysics® Simulation

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Abstract

Ultrasound as an advanced oxidation process (AOP) has been shown to effectively destruct organic and inorganic contaminants in aqueous solution [1]. In the sonicated solution, collapse of cavitation bubbles generates localized "hot spots" where temperature and pressure are as high as 5,000 K and 1,000 atm, respectively [2]. In this extreme condition, thermolysis and OH oxidation are two mechanisms for the contaminant degradation [1, 2]. Although ultrasound technology shows great potential in the AOP, the commonly-used ultrasound irradiator (e.g., horn type) generates a localized cavitation and a non-uniform cavitation field, which makes it difficult to scale-up the AOP with the typical horn irradiator [3]. Therefore, a novel configuration design of an ultrasound irradiator is necessary to maximize the cavitation-induced chemical effects for large-scale AOP.

When expecting efficiency and economics in the design of a large-scale system for AOP, computational simulation seems more attractive if it provides compatible results to real measurements. The computational simulation can easily investigate different reactor geometries, irradiator configurations, and ultrasound frequencies to optimize the design. COMSOL Multiphysics® has been applied to simulate acoustic field and sonochemistry in reactors [4,5,6]. The characterization of a design becomes much simpler and straightforward with the aid of computational simulation.

In this study, COMSOL was used to characterize an ultrasound irradiator design, in which there were a transducer, an ultrasound irradiator (20 kHz, 2.6 – 3.8 cm in diameter, and 28.0 cm in length), and a water tank (with dimensions of 61.0 cm × 61.0 cm × 45.0 cm and a volume of 167.5 L) involving different physical phenomena. The piezoelectric material in the transducer converts electrical energy to mechanical vibration, which then passes through the ultrasound irradiator and is intensified at the end of the irradiator. Then the irradiator emits the amplified mechanical waves (ultrasound waves) in water, and those waves propagate in the water tank radially.

The simulation was established as a 2D axisymmetric geometry. The physics "acoustic-piezoelectric interaction" was selected in a frequency domain study. "Pressure acoustics", "piezoelectric material", and "linear elastic material models" were correspondingly set for water,

transducer, and ultrasound irradiator domains. Boundary conditions for surfaces in contact with air were set to "free", whereas surfaces in contact with water were defined as acoustic-structure boundaries. In addition, "cylindrical wave radiation" was chosen for the acoustics boundary condition because the ultrasound irradiator has cylindrical pieces with different diameters. "Free triangular" was selected with appropriate maximum element size to mesh each domain.

The simulated acoustic pressure field surrounding the designed ultrasound irradiator is consistent to experimental measurements [7], shown in Figure 1 (2D) and Figure 2 (3D). The computed results have showed that the ultrasound irradiator design with a serial-stepped configuration improved cavitation effects as compared to typical horn irradiators generating a localized cavitation. COMSOL seems to be a reliable and convenient tool for such scale-up designs of ultrasound irradiators for AOP.

Reference

[1] L.K. Weavers et al., Aromatic compound degradation in water using a combination of sonolysis and ozonolysis, Environmental Science and Technology, 32, 2727-2733 (1998).
[2] K.S. Suslick, The chemical effects of ultrasound, Scientific American, 260, 80-86 (1989).
[3] T.J. Mason; A. Tiehm, Advances in sonochemistry, Volume 6: Ultrasound in environmental protection, Connecticut: Jai Press (2001).
[4] J. Klima et al., Optimisation of 20 kHz sonoreactor geometry on the basis of numerical simulation of local ultrasonic intensity and qualitative comparison with experimental results, Ultrasonics Sonochemistry, 14, 19-28 (2007).
[5] L. Csoka et al., Comparison of cavitational activity in different configurations of sonochemical reactors using model reaction supported with theoretical simulations, Chemical Engineering Journal, 178, 384-390 (2011).
[6] F.J. Trujillo; K. Knoerzer, A computational modeling approach of the jet-like acoustic streaming and heat generation induced by low frequency high power ultrasonic horn reactors, Ultrasonics Sonochemistry, 18, 1263-1273 (2011).
[7] Z. Wei et al., Designing and characterizing a serial stepped ultrasonic horn for enhanced acoustic cavitation, Ultrasonics Sonochemistry (in preparation).

Figures used in the abstract

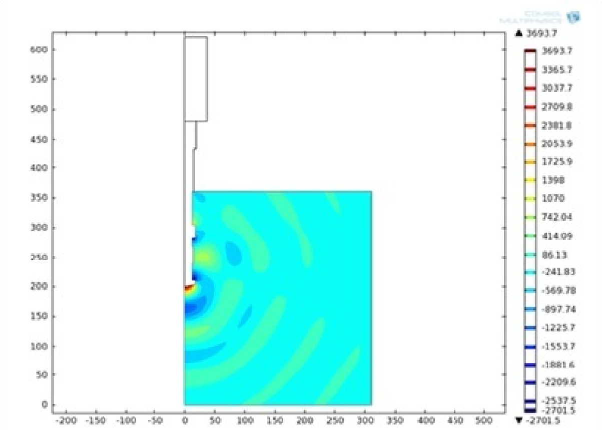

Figure 1 Simulated Results of Acoustic Pressure Distribution in 2D
(units for axis and color bar are mm and Pa, respectively)

Figure 1: Simulated Results of Acoustic Pressure Distribution in 2D (units for axis and color bar are mm and Pa, respectively).

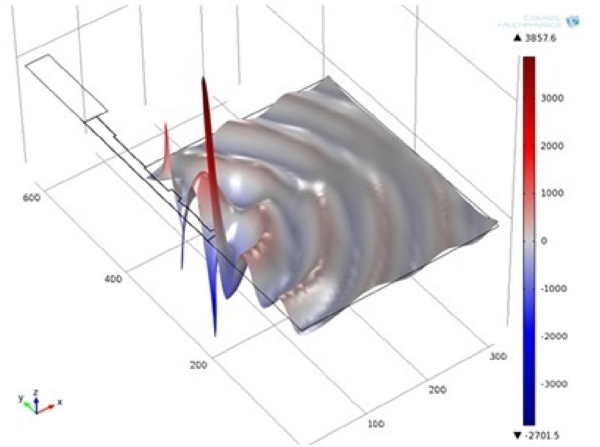

Figure 2 Simulated Results of Acoustic Pressure Distribution in 3D
(units for axis and color bar are mm and Pa, respectively)

Figure 2: Simulated Results of Acoustic Pressure Distribution in 3D (units for axis and color bar are mm and Pa, respectively).