**MODELLING OF ACOUSTIC-BASED BATCH SONOCHEMICAL REACTORS**

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**ABSTRACT**

Ultrasound is known to initiate and intensify chemical reactions. In recent years the chemical engineering community has shown growing interest towards the use of high-power low-frequency ultrasound for industrial process intensification, since ultrasound based reactors are macroscopically characterized by mild temperatures. Intense research interest within sonochemistry is shown towards wastewater cleaning1.

The chemical effects of ultrasound are attributed to the induced cavitation of the liquid. Briefly, the rarefraction phase of an ultrasound wave induces fractures in the liquid forming localized voids whereas the compression phase induces a violent collapse2. The pressure amplitute required for a liquid to cavitate is called Blake threshold and we can assume based on experiments that for a non preprocessed water 3 the Blake threshold is 1 atm4. The cavitational collapse is accompanied by the creation of a hot spot in the liquid enhancing reaction efficiency through the formation of radicals and heat diffusion5. Even though the mechanism of acoustic cavitation remains to be fully elucidated, sonoreactors are already seeing insudtrial use and full parameter optimization is needed, which can be achieved through modelling and pilot reactor testing.

Motivated by this, we constructed a numerical simulation approach of phenol degradation through radical formation in an ultrasound batch reactor that captures the spatiotemporal complexities associated with the periodic forcing of the liquid. Furthermore, the wave propagation manifesting in this bubbly liquid alters the wave attenuation coefficient due to the compressibility of the gaseous phase. The total volume occupied by these bubbles is termed void fraction or bubble cluster. Void fraction is linearly dependent on pressure amplitude6. Thus, the attenuation coefficient was adjusted considering bubble cluster formation and gas compressibility7. The regions of the liquid that reached the Blake threshold were assumed to cavitate and were integrated in the reaction rate calculation through an Arrhenius-type equation.

Our findings, in constistence with literature8, show that bubbly liquids heavily attenuate wave propagation. The magnitude of the void fraction ranged between 10-3 near the transducer to 0 when the pressure amplitude fell below atmospheric pressure. Furthermore, our model predicts that phenol concentration is time and sonicator power dependent.

**KEYWORDS:** Sonoreactors, Modelling, Cavitation

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