Sonochemical Reactor Optimization using Computational Acoustics Techniques

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Abstract: This paper proposes a computational technique able to predict the cavitation zone in a low frequency (20 kHz) sonochemical reactor. The purpose of such a tool is to support the design of more efficient sonochemical reactors.

PROBLEM DEFINITION

The designer of a sonochemical reactor is confronted to a complex problem characterized by a large number of design parameters: reactor shape and dimensions, number, positions and power of ultrasound sources, frequency, solvant, temperature etc. A wide parametric study cannot be conducted experimentally due to time and cost constraints and a numerical model seems the only viable approach. Such a model must reflect the inherent complexity of the system and at the same time be simple enough to provide relevant results in a reasonable amount of time. The model is based on the following components: (1) a finite element model solving the Helmholtz equation in the fluid, (2) a relationship between the local sound intensity and the volume fraction of cavitation bubbles (3) equivalent acoustic properties (density and sound celerity) of the cavitating media (4) the Nyborg model of acoustic streaming. Each of these components is briefly described below and the paper is concluded by a discussion of a typical result.

SOUND FIELD IN THE REACTOR

We assume that the sound field in the reactor obeys the Helmholtz equation and that non-linear effects can be represented by a dependency of the sound speed on the sound pressure field:

\[ \nabla^2 p + \left( \omega/c(p) \right)^2 p = 0 \]  

A solution to this equation in the fluid domain is sought by the finite element method first introduced in acoustics by Craggs then popularized in general purpose computational acoustics programs like SYSNOISE. The dispersion relation requires a non-linear solution scheme: (1) the initial solution \( p_0 \) is obtained with \( k = \omega c \) where \( c \) is the sound celerity in the non-cavitating fluid then (2) new solutions \( p_i \) are iteratively obtained by the recurrence:

\[ \nabla^2 p_i + \left( \omega/c(p_{i-1}) \right)^2 p_i = 0 \]  

At each iteration, a tentative cavitation zone is defined by comparing the local pressure with the asymptotic Blake threshold \( p_B = p_0 - p_v \) where \( p_0 \) is the atmospheric pressure and \( p_v \) the vapour pressure. If the local pressure is higher than \( p_B \), cavitation occurs and one can estimate the volume fraction of the gas \( \Omega \) using a relation proposed by Ciuti which linearly relates \( \Omega \) to the difference between the local sound intensity \( I \) and the intensity threshold \( I_t \):

\[ \Omega = b(I - I_t) \]  

Equivalent properties for the cavitating medium are then calculated from the gas volume fraction using one of the numerous models published in the literature, for instance the model described in Wood's textbook:

\[ \rho_g = \frac{1}{\rho_0 + \Omega \left( \frac{1}{\rho_g} - \frac{1}{\rho_0} \right)} \]  

\[ c_g = c_0 \left[ 1 + \Omega \left( \frac{\rho_0 c_0^2}{\rho_g c_g^2} \right) \right]^{-\frac{1}{2}} \]
where the subscripts $R$, $O$ and $g$ refer respectively to the cavitating fluid, the liquid phase and the gas phase. More complex models\textsuperscript{6,7} will be implemented and tested in the near future.

RESULTS

The model has been used to predict the cavitation zone in a cylindrical tank under the assumption of a perfectly axisymmetric sound field induced by a centered acoustic horn emitting at 20 kHz. The tank is filled with water.

![Image](image.png)

**FIGURE 1.** Cavitation zone for three different sound intensity

The cavitation zone near the horn tip correlates well with measured bubble clouds; the extension of the cavitation zone along the axis of the reactor is not found experimentally and can most probably be explained by an underestimation of the sound absorption in the fluid.

CONCLUSIONS AND POSSIBLE EXTENSIONS

The proposed model gives qualitatively good predictions of the extent of the cavitation area in a sonochemical reactors and can be easily extended to predict the streaming pattern indeed, the sound field being known, it is easy to calculate the streaming forces\textsuperscript{8} and inject them in any standard CFD code to predict the streaming pattern. The calculation time of a finite element scheme increases with the $7^{th}$ power of the frequency so that this modeling technique is limited, for all practical purpose, to low frequency sonochemical reactors (~20-100 kHz). The current model could certainly be refined by replacing the gas volume fraction $\omega$ by the actual bubble distribution function $\Omega$ for which a conservation equation has been recently proposed\textsuperscript{9}.

REFERENCES

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