Scale-up Design of Ultrasound Horn for Advanced Oxidation Process Using COMSOL Simulation

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OUTLINE

1. Background
2. Objectives
3. Simulation
4. Results
5. Future Work
Ultrasound (>20kHz)

Cavitation

Emulsifying, Synthesis, Imaging, Damage Detection, cleaning ... 

- Organic pollutants
  - polycyclic aromatic hydrocarbon
- Inorganic pollutants
  - arsenic
- Disinfection
  - reduce chemical addition
- Desorption
  - enhanced oil recovery

$T \approx 5000 \text{ K}$

$H_2O \rightarrow \cdot H + \cdot OH$

(Suslick, 1989)

(Moussatov et al., 2003)
Typical ultrasonic horn

- Localized cavitation
- Low energy efficiency — 8-29%\textsuperscript{a}
- Scaling-up is very difficult

\textsuperscript{a} Contamine et al., 1994; Kimura et al., 1996; Weavers et al., 2000; Bhirud et al., 2004; Pee, 2008; Thangavadivel et al., 2009.
Objectives

• Improved horn configuration – Enhanced cavitation

• COMSOL – Tool
  – Piezoelectric material model
  – Linear elastic material model
  – Pressure acoustics model

a — typical horn; b — designed horn
Design Verification

Pressure

Cavitation

Removal
Experimental Characterization

- **Hydrophone Measurements**
  - *a device that can record underwater sound by receiving pressure signals*

- **Sonochemiluminescence (SCL)**

\[ \text{Luminol} + \cdot \text{OH} \rightarrow \text{Product} + h\nu \]
Experimental Results

Energy efficiency increased to 31.5%
Summary

- More energy-emitting surfaces
- Multiple reactive zones
- Higher energy efficiency

COMSOL
- Comparable results
- A reliable design tool
Large-Scale Evaluation

2D and 3D acoustic pressure distribution in the water tank
Future Work

• Large-volume reactor

• Flow cell reactor

• Array of designed horns

• Sediment treatment
Acknowledgement

• The COMSOL Conference
• Dr. Linda Weavers, Dr. John Lenhart, Dr. Ruiyang Xiao, Dr. Meiqiang Cai, Dr. Chin-Min Cheng, Matthew Noerpel, and Mengling Stuckman
Questions?
Governing Equations

• Piezoelectric material model for transducer

\[
\begin{align*}
\text{Stress} - \text{charge} & \quad \begin{cases} 
T = c_E S - e^T E \\
D = e S + \varepsilon_S E
\end{cases} \\
\text{Strain} - \text{charge} & \quad \begin{cases} 
S = s_E S + d^T E \\
D = d T + \varepsilon_T E
\end{cases}
\end{align*}
\]

• Linear elastic material model for irradiator

\[-\rho \omega^2 u - \nabla \cdot \sigma = F_V e^{i\phi}\]

• Pressure acoustics model for water

\[\nabla^2 P - \frac{1}{c^2} \frac{\partial^2 P}{\partial t^2} = 0\]
Physical Characterization – Hydrophone

volts $\propto$ pressure
Physical Characterization – Sonochemiluminescence (SCL)

$Luminol + \cdot OH \rightarrow Product + h\nu$

Typical horn
Energy

\[ P_{ac} = (dT/dt) \times C_p \times M \]

<table>
<thead>
<tr>
<th>Ultrasonic horn</th>
<th>Freq. (kHz)</th>
<th>Electrical power input (W)</th>
<th>Reaction volume (mL)</th>
<th>Emitting area (cm²)</th>
<th>Acoustic power (W)</th>
<th>Power intensity (W cm⁻²)</th>
<th>Power density (W L⁻¹)</th>
<th>Energy efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Designed</td>
<td>20</td>
<td>1000</td>
<td>1250</td>
<td>134</td>
<td>315</td>
<td>2.35</td>
<td>252</td>
<td>31.5</td>
</tr>
<tr>
<td>Typical (Branson) (^a)</td>
<td>20</td>
<td>350</td>
<td>50</td>
<td>1.20</td>
<td>66.5</td>
<td>55.8</td>
<td>1340</td>
<td>19.0</td>
</tr>
<tr>
<td>Typical (Fisher Scientific) (^b)</td>
<td>20</td>
<td>275</td>
<td>60</td>
<td>1.20</td>
<td>25.8</td>
<td>21.5</td>
<td>430</td>
<td>9.38</td>
</tr>
</tbody>
</table>

\(^a\) Weavers et al., 2000

\(^b\) Pee, 2008

\(^c\) Contamine et al., 1994; Kimura et al., 1996; Weavers et al., 2000; Bhirud et al., 2004; Pee, 2008; Thangavadivel et al., 2009.

8 – 29% \(^c\)
Cavitation

\[ TA + \cdot OH \rightarrow HTA \]

\[ k_{nor} = k_{th} \times (PD_{dh}/PD_{th}) \]

- \( k_{nor} \) — normalized rate (\( \mu M \text{ min}^{-1} \))
- \( k_{th} \) — rate constant for typical horn (\( \mu M \text{ min}^{-1} \))
- \( PD_{dh} \) — power density for designed horn (W)
- \( PD_{th} \) — power density for typical horn (W)

<table>
<thead>
<tr>
<th>Ultrasonic horn</th>
<th>HTA formation rate (( \mu M \text{ min}^{-1} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Designed</td>
<td>0.36</td>
</tr>
<tr>
<td>Typical (Sonics &amp; Materials)(^b)</td>
<td>0.08</td>
</tr>
<tr>
<td>Typical (Fisher Scientific)(^c)</td>
<td>0.18</td>
</tr>
</tbody>
</table>

\(^a\) Weavers et al., 2000
\(^b\) Price and Lenz, 1993
\(^c\) He, 2006

- Initial water temperature for experiment a is 20°C;
- Electrical power input is 500 W
Naphthalene Degradation

\[ \text{Naphthalene} + \cdot \text{OH} \rightarrow \text{Products} \]

\[ k_{nor} = k_{th} \times \left(\frac{PD_{dh}}{PD_{th}}\right)^a \]

\[^a\text{Weavers et al., 2000}\]
Large-Scale Application

- Water tank setup

Diagram of experimental setup for hydrophone measurements in plexiglas box (the depth tangential to horn tip is defines z = 0; 1—Branson 902R Model transducer; 2—serial stepped ultrasonic horn; 3—Reson T4013 hydrophone; 4—water; 5—plexiglas box)
Large-Scale Evaluation

Transducer (PZT-5H) - piezoelectric material model
Horn irradiator (stainless steel) - linear elastic material model
Tank (water) - pressure acoustics model
Large-Scale Application

3D (left) and contour (right) mapping of hydrophone measurements in plexiglas tank

(X-Y plane at $z = 0$ cm)
Large-Scale Application

3D (left) and contour (right) mapping of hydrophone measurements in plexiglas tank

(X–Y plane at \( z = +4 \) cm)
Large-Scale Application

3D (left) and contour (right) mapping of hydrophone measurements in plexiglas tank
(X–Y plane at \( z = -4 \text{ cm} \))
Chemical Structure

Naphthalene

Ethylenediaminetetraacetic Acid (EDTA)
Schematic diagram of longitudinal vibration of single step horn and its equivalent circuits

\[
\begin{align*}
F_2 &= \alpha_{21} \ddot{\xi}_1 + \alpha_{22} F_1 \\
\dot{\xi}_2 &= \alpha_{11} \ddot{\xi}_1 + \alpha_{12} F_1
\end{align*}
\]

\[
\begin{bmatrix}
\dot{\xi}_2 \\
F_2
\end{bmatrix} =
\begin{bmatrix}
\alpha_{11} & \alpha_{12} \\
\alpha_{21} & \alpha_{22}
\end{bmatrix}
\begin{bmatrix}
\ddot{\xi}_1 \\
F_1
\end{bmatrix}
\]

\[
A_i =
\begin{bmatrix}
\alpha_{11}^i & \alpha_{12}^i \\
\alpha_{21}^i & \alpha_{22}^i
\end{bmatrix}
\]

\[
A = A_1 A_{i-1} \cdots A_2 A_i
\]

\[
A =
\begin{bmatrix}
\alpha_{11} & \alpha_{12} \\
\alpha_{21} & \alpha_{22}
\end{bmatrix}
\]

\[
(A)
\]

\[
(b)
\]
Diagram of experimental set-up