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

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Boston, MA

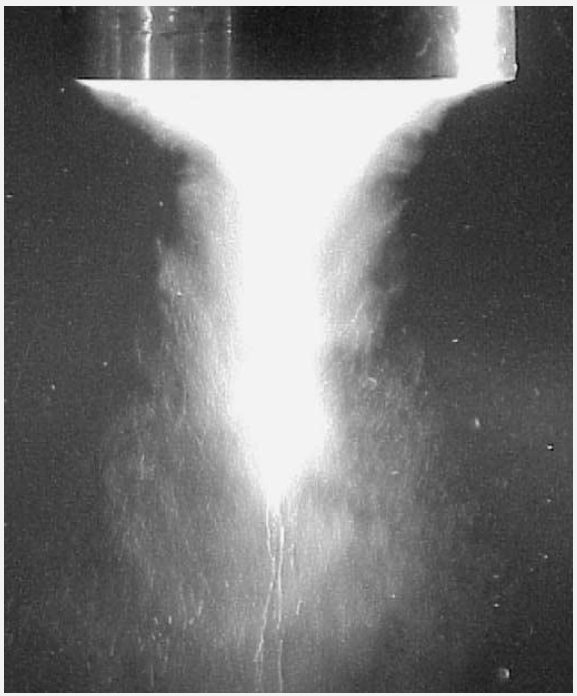
OUTLINE

1. Background
2. Objectives
3. Simulation
4. Results
5. Future Work

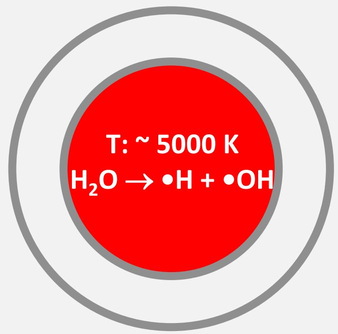
Ultrasound (>20kHz)

Emulsifying, Synthesis, Imaging, Damage Detection, cleaning …

Cavitation



(Moussatov et al., 2003)



(Suslick, 1989)

- Organic pollutants
  – *polycyclic aromatic hydrocarbon*
- Inorganic pollutants
  – *arsenic*
- Disinfection
  – *reduce chemical addition*

- Desorption
  – *enhanced oil recovery*

Typical ultrasonic horn

- **Localized cavitation**
- **Low energy efficiency**
  - **8-29%[a]**
- **Scaling-up is very difficult**

[a] Contamine et al.,1994; Kimura et al., 1996; Weavers et al., 2000; Bhirud et al., 2004; Pee, 2008; Thangavadivel et al., 2009.

Objectives

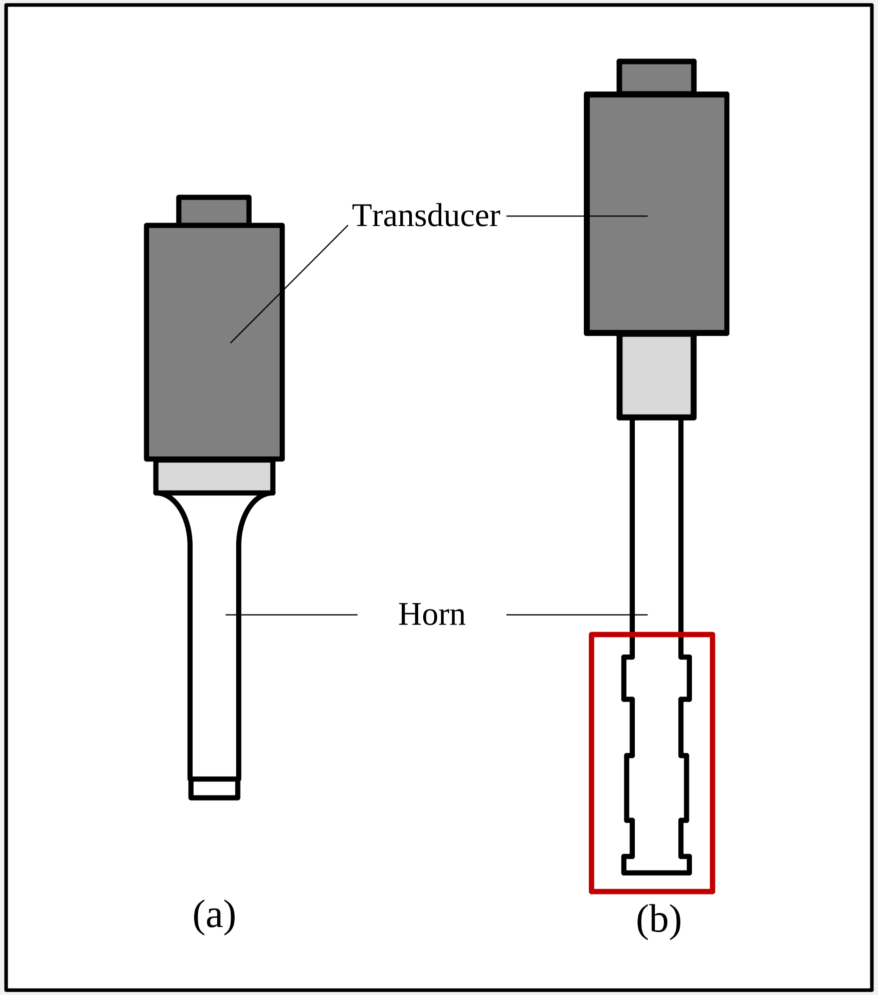
- Improved horn configuration – Enhanced cavitation

- COMSOL – Tool

  – Piezoelectric material model

  – Linear elastic material model

  – Pressure acoustics model



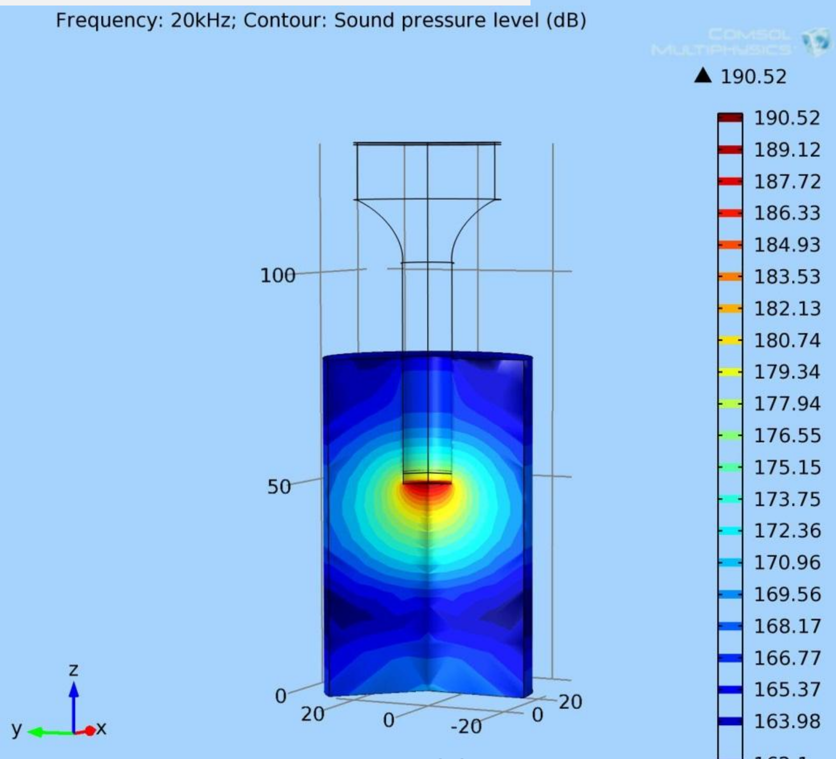
a —typical horn; b — designed horn

Design Verification

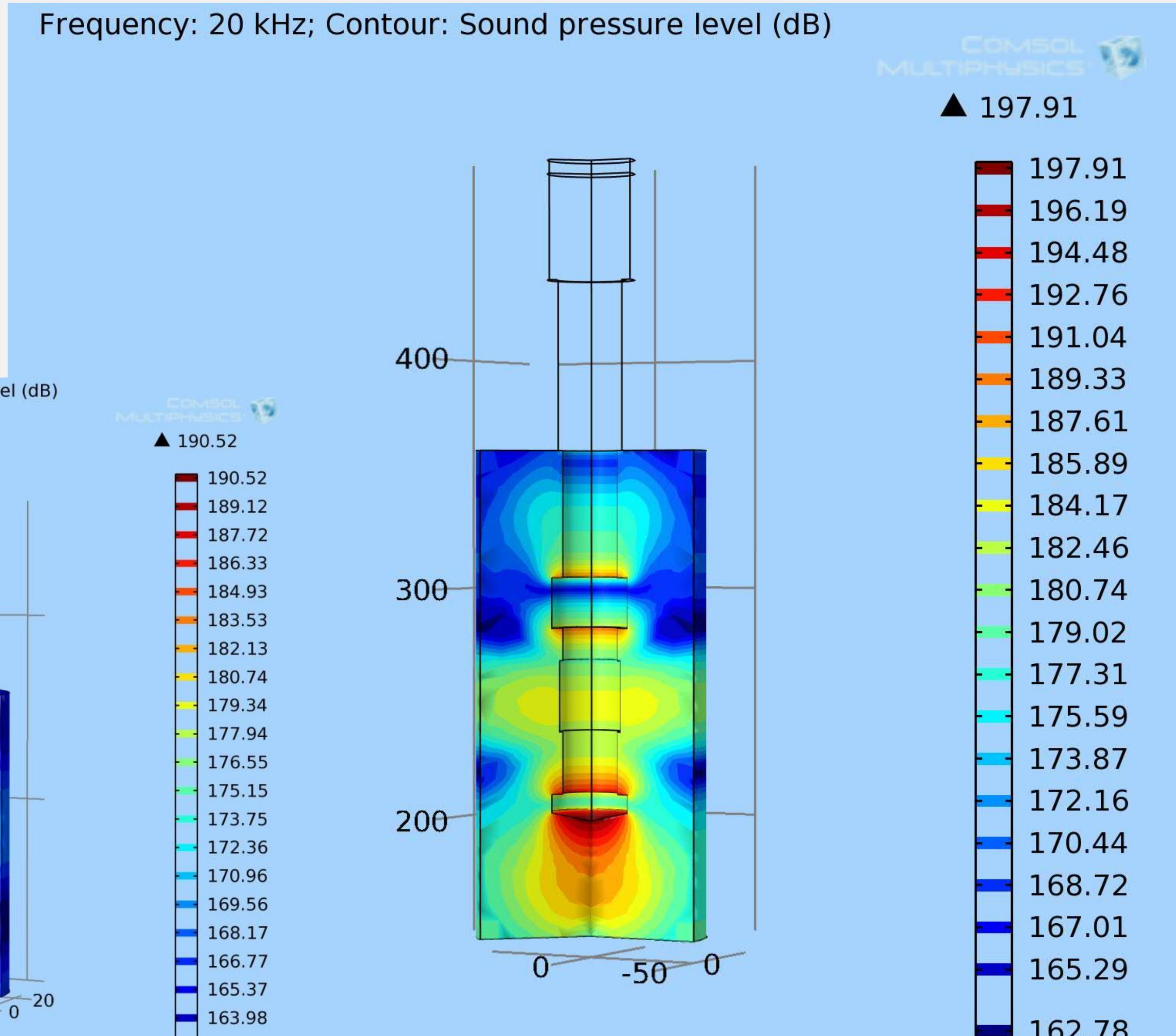
Pressure ↑

Cavitation ↑

Removal ↑



Typical horn

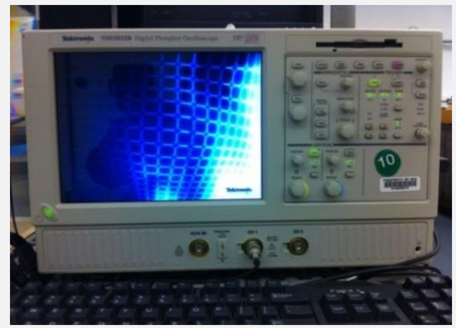


Designed horn

Experimental Characterization

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

Reson TC4013 Hydrophone



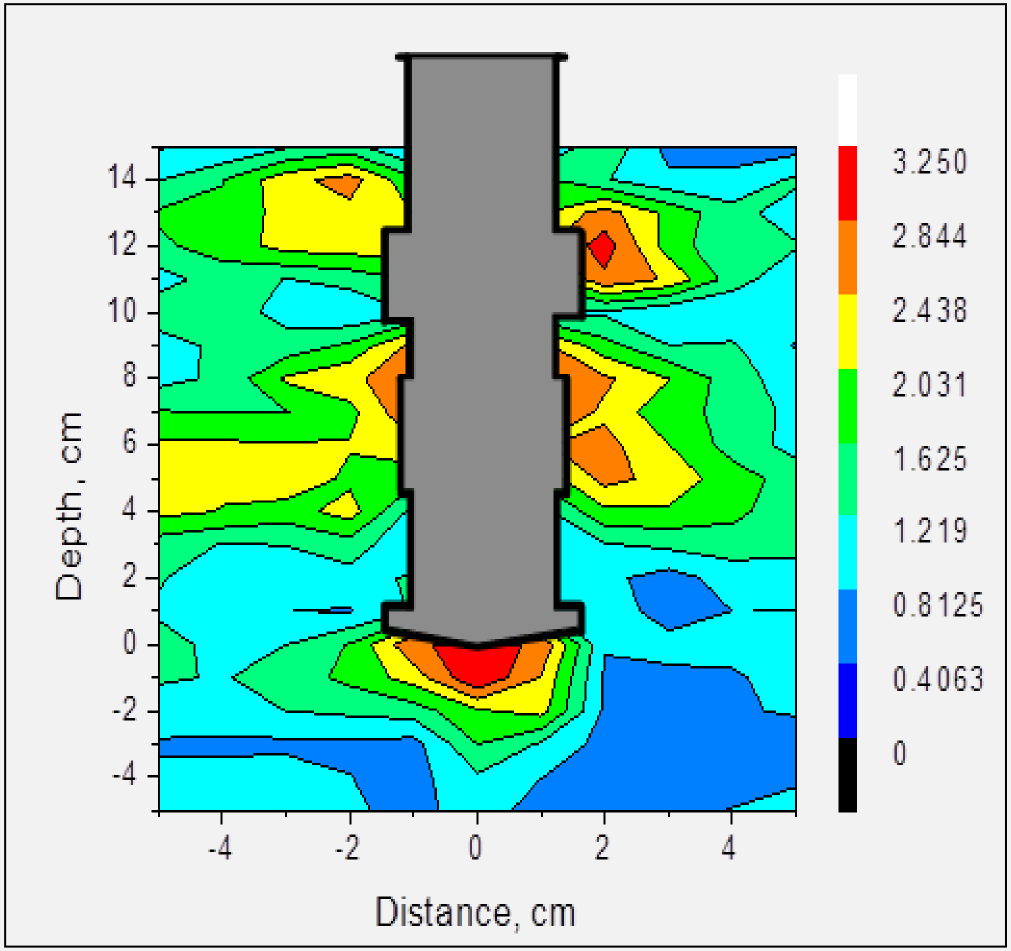
TDS 5000 Tektronix oscilloscope

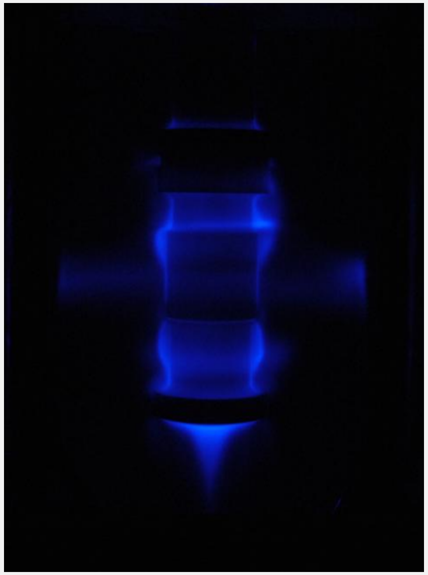
- Sonochemiluminescence (SCL)

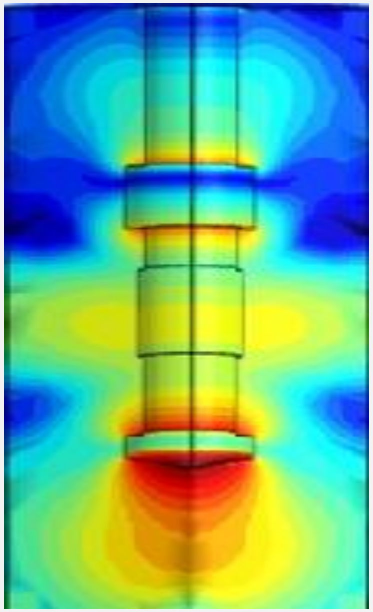
$$Luminol + \cdot OH \rightarrow Product + hv$$

Distribution and Location

Experimental Results







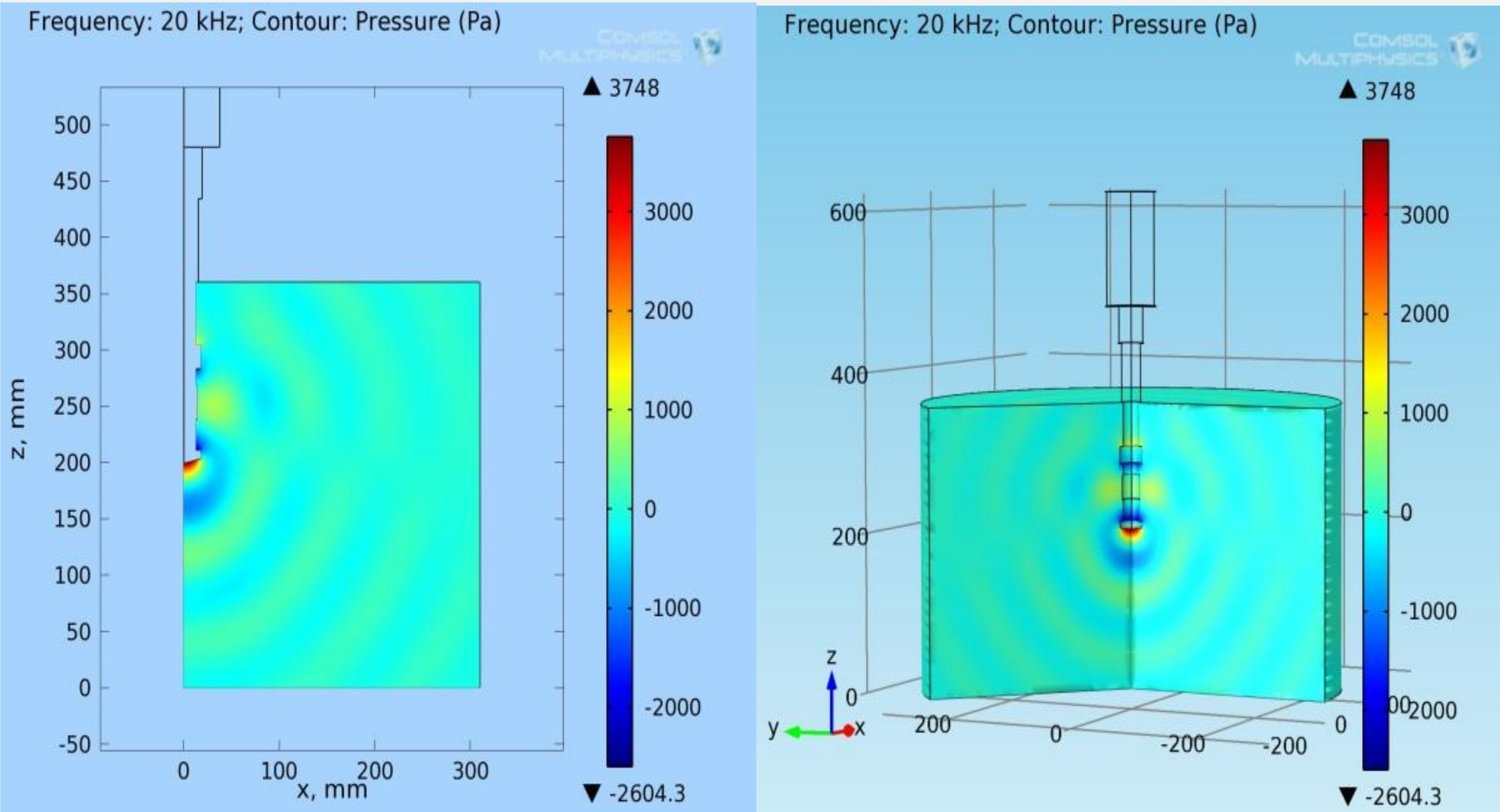
Energy efficiency increased to 31.5%

Summary

- More energy-emitting surfaces
- Multiple reactive zones
- Higher energy efficiency
- COMSOL
  - *Comparable results*
  - *A reliable design tool*

} Large Scale

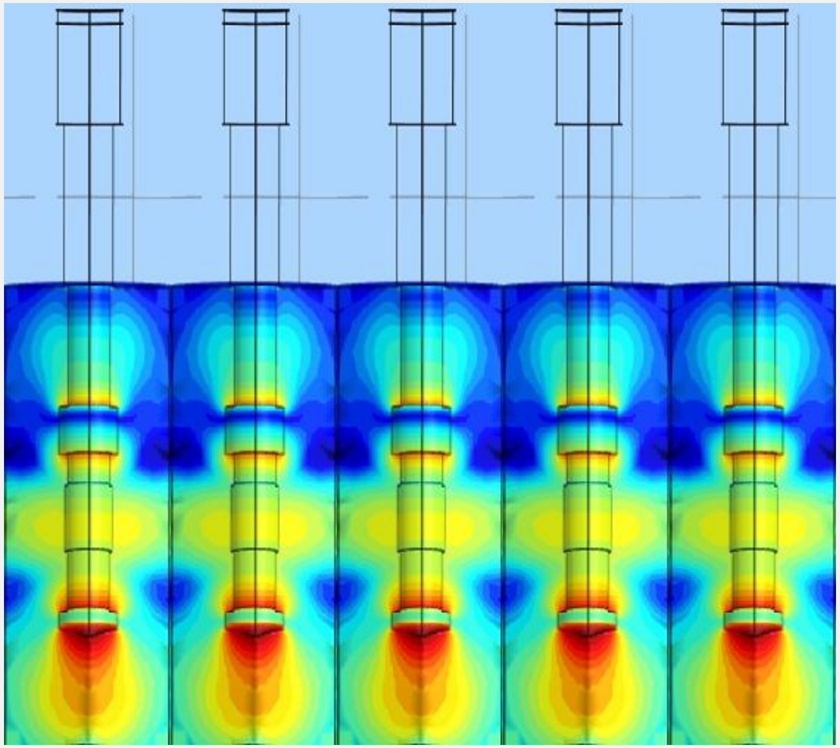
Large-Scale Evaluation



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

Future Work

- Large-volume reactor
- Flow cell reactor
- Array of designed horns
- Sediment treatment

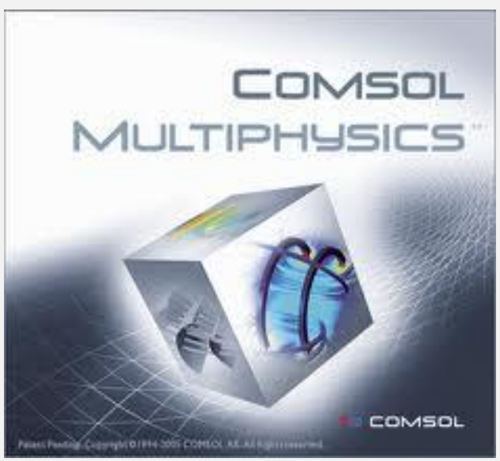


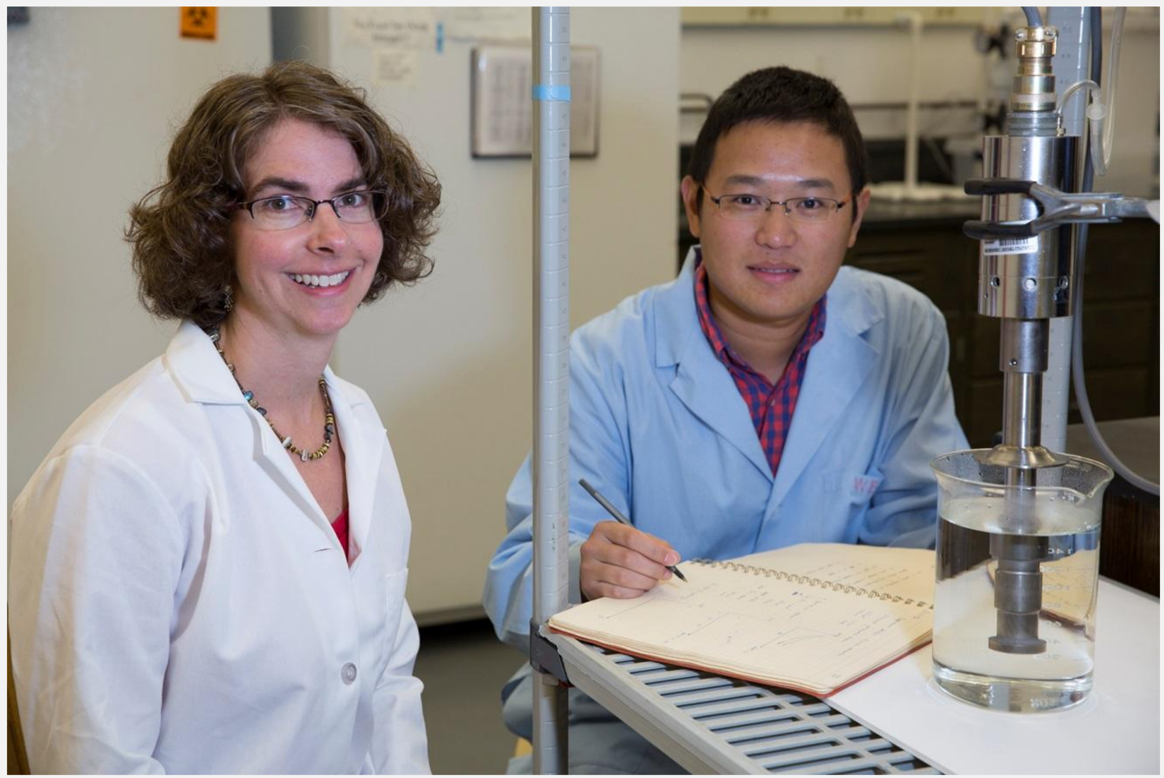
COMSOL

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

COMSOL CONFERENCE BOSTON 2013





Questions?

Governing Equations

- Piezoelectric material model for transducer

$$Stress-charge \quad \begin{cases} \boldsymbol{T} = c_E\boldsymbol{S} - e^T\boldsymbol{E} \\ \boldsymbol{D} = e\boldsymbol{S} + \varepsilon_S\boldsymbol{E} \end{cases}$$

$$Strain-charge \quad \begin{cases} \boldsymbol{S} = s_E\boldsymbol{S} + d^T\boldsymbol{E} \\ \boldsymbol{D} = d\boldsymbol{T} + \varepsilon_T\boldsymbol{E} \end{cases}$$

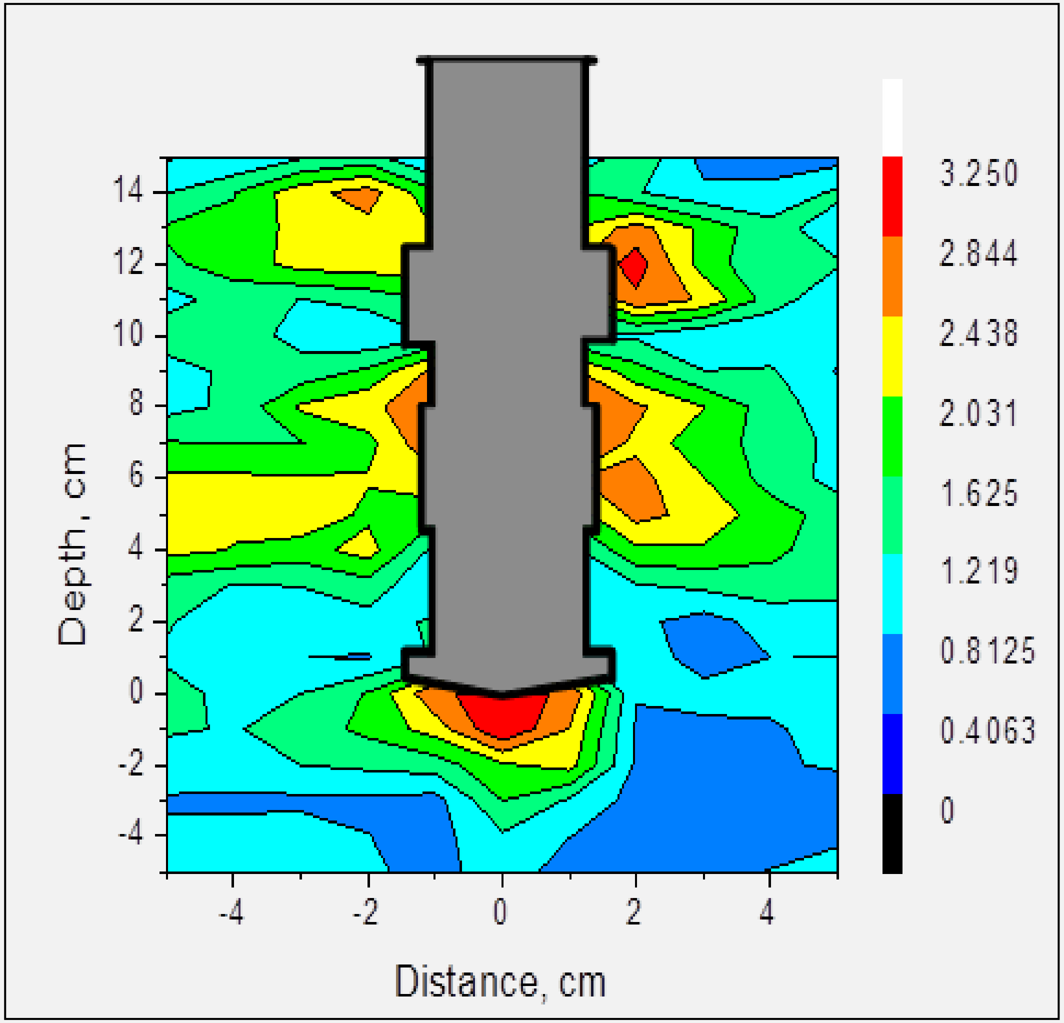
- Linear elastic material model for irradiator

$$-\rho\omega^2\boldsymbol{u} - \nabla\cdot\sigma = \mathbf{F}_V e^{i\phi}$$

- Pressure acoustics model for water

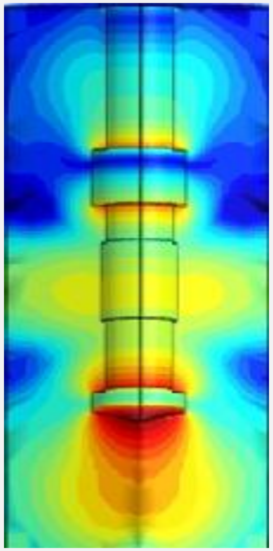
$$\nabla^2 P - \frac{1}{c^2}\frac{\partial^2 P}{\partial t^2} = 0$$

Physical Characterization – Hydrophone

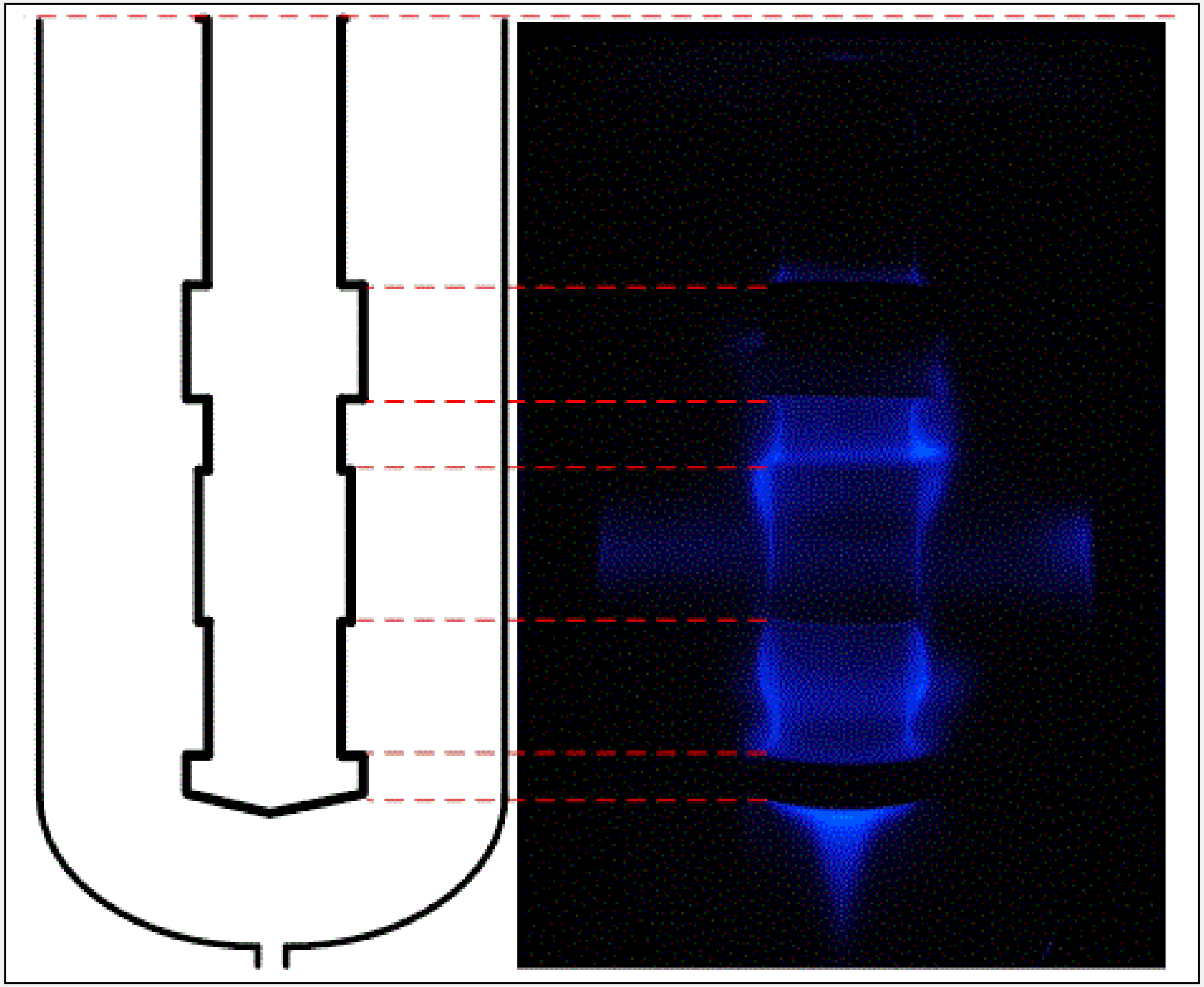


volts ∝ pressure

Ultrasonic reactor



Physical Characterization – Sonochemiluminescence (SCL)



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

Typical horn

Energy

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

Ultrasonic horn	Freq. (kHz)	Electrical power input (W)	Reaction volume (mL)	Emitting area (cm^2)	Acoustic power (W)	Power intensity (W cm^{-2})	Power density (W L^{-1})	Energy efficiency (%)
Designed	**20**	**1000**	**1250**	**134**	**315**	**2.35**	**252**	**31.5**
Typical (Branson) [a]	20	350	50	1.20	66.5	55.8	1340	19.0
Typical (Fisher Scientific) [b]	20	275	60	1.20	25.8	21.5	430	9.38

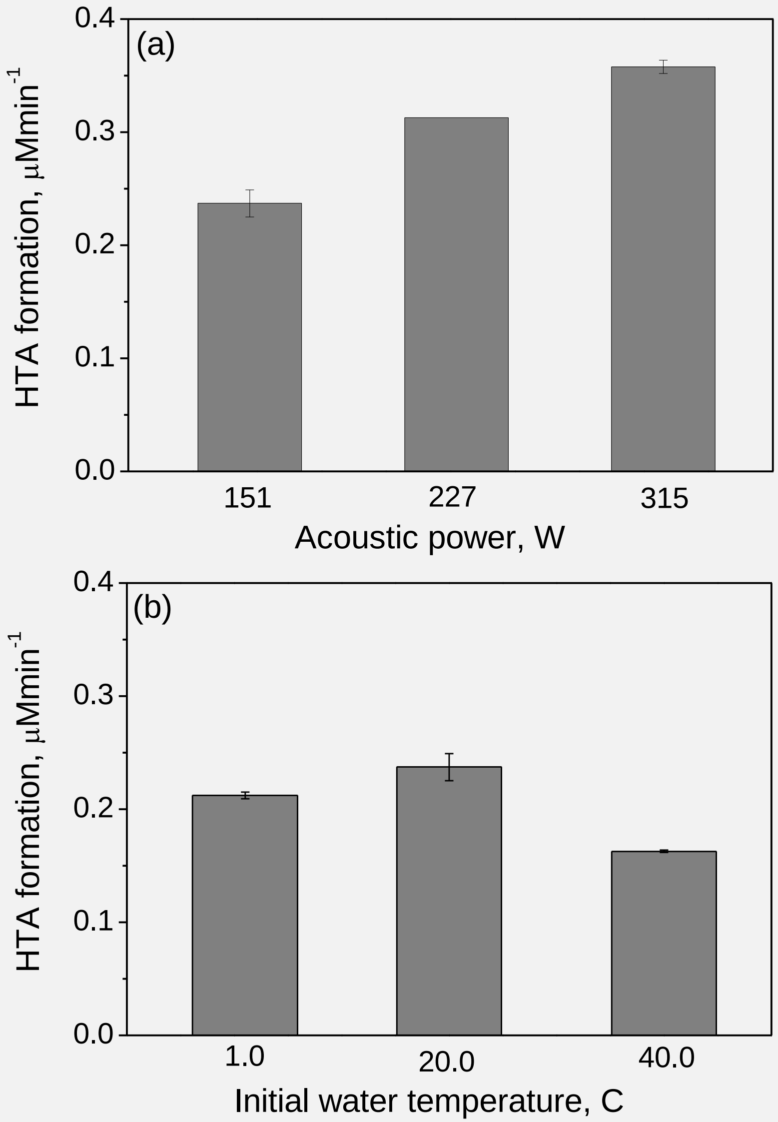
8 – 29% [c]

[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.

Cavitation



a — initial temperature for experiment a is 20ºC;
b — electrical power input is 500 W

$$TA + \cdot OH \rightarrow HTA$$

$$k_{nor} = k_{th} \times (PD_{dh}/PD_{th})\ ^{a}$$

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

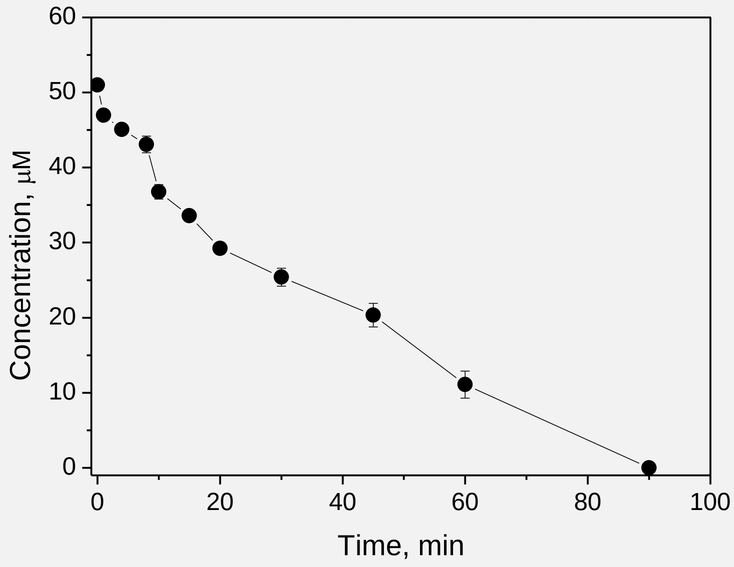
Ultrasonic horn	HTA formation rate (μM min^{-1})
Designed	**0.36**
Typical (Sonics & Materials) [b]	0.08
Typical (Fisher Scientific) [c]	0.18

[a] Weavers et al., 2000

[b] Price and Lenz, 1993

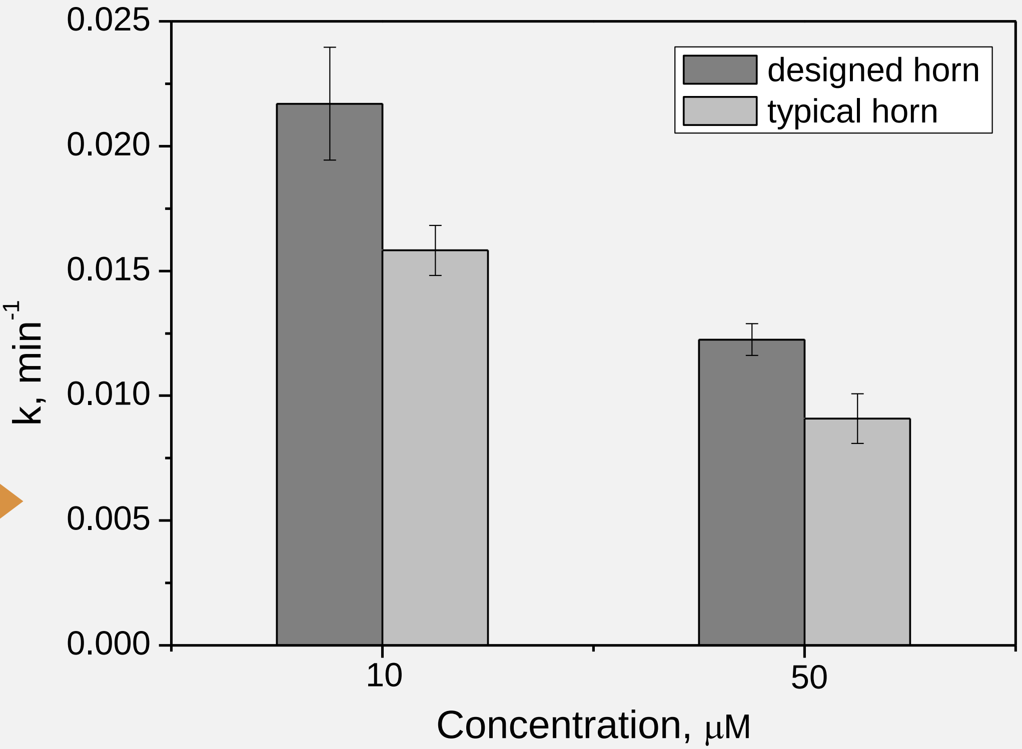
[c] He, 2006

Naphthalene Degradation



$$Naphthalene + \cdot OH \rightarrow Products$$

$$k_{nor} = k_{th} \times (PD_{dh}/PD_{th})^{a}$$



[a] Weavers et al., 2000

Large-Scale Application

- Water tank setup

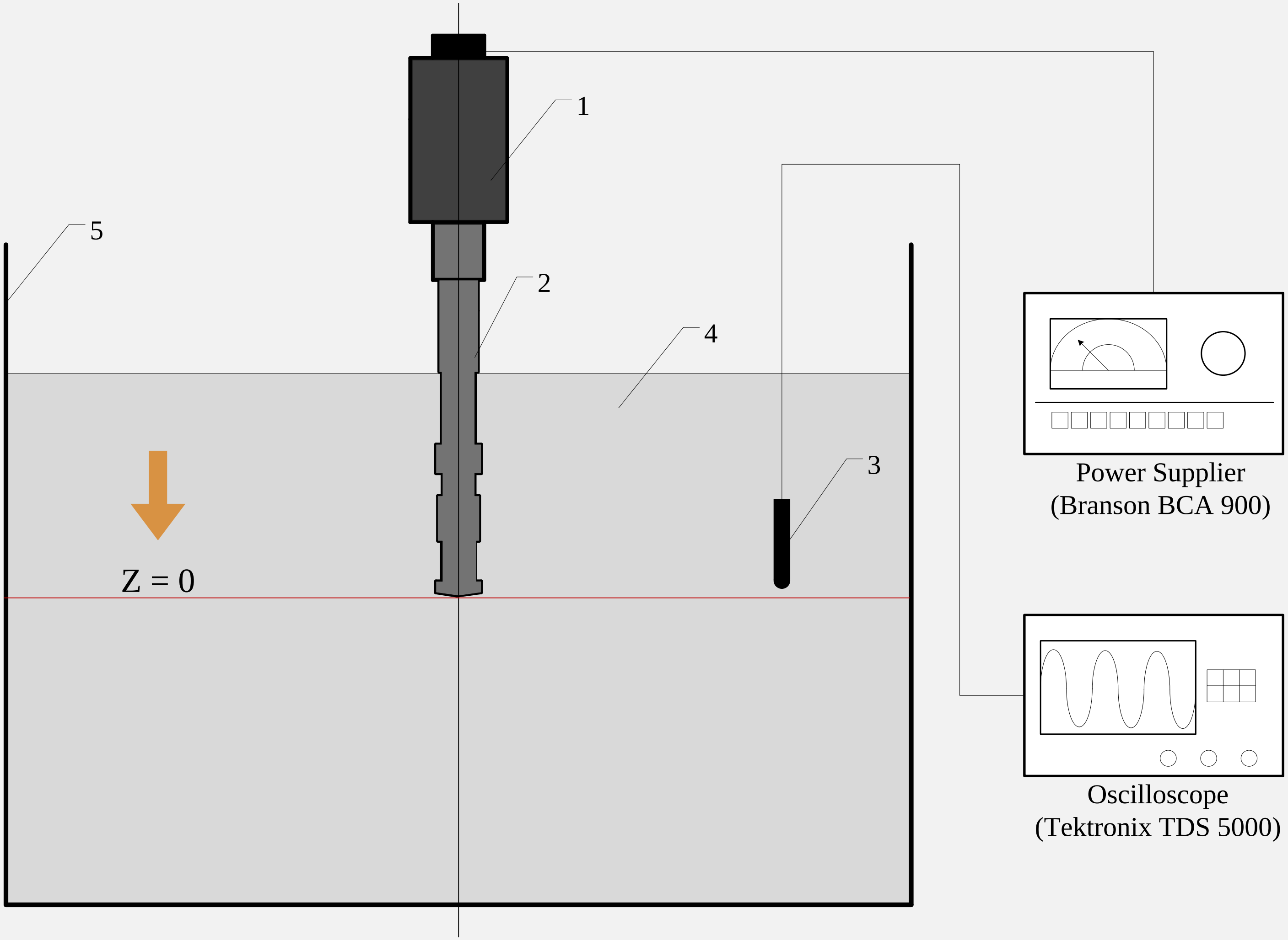
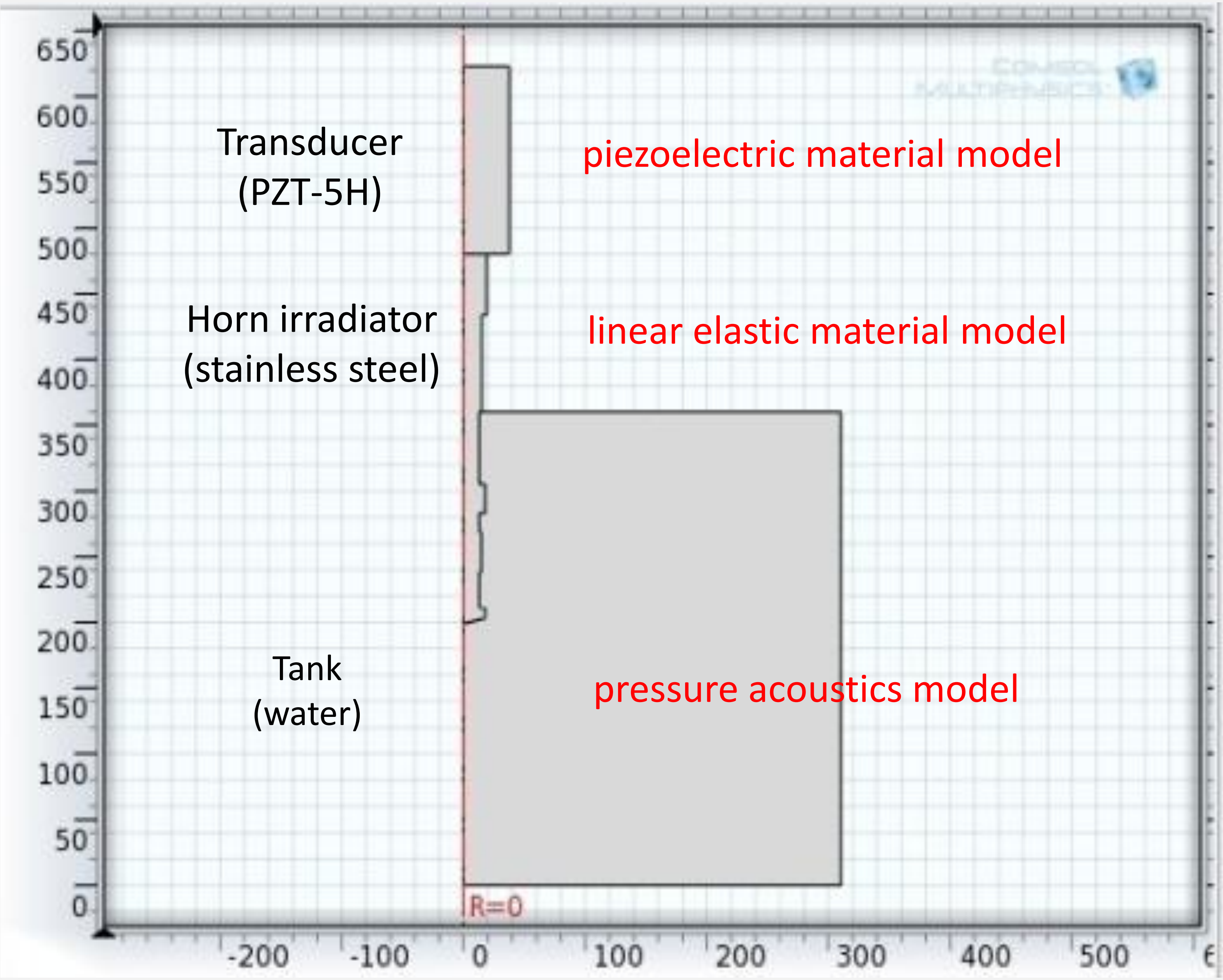
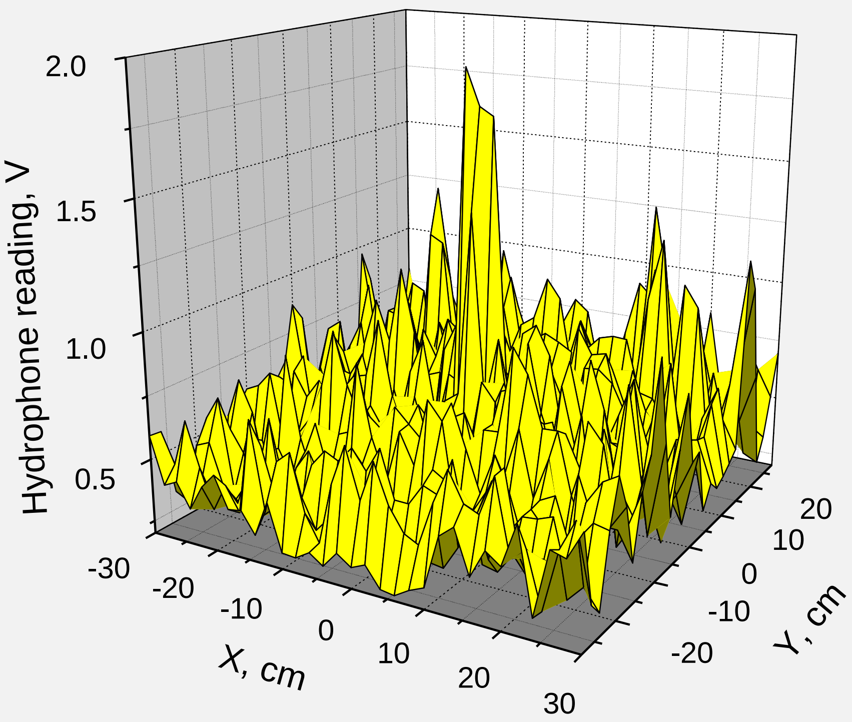


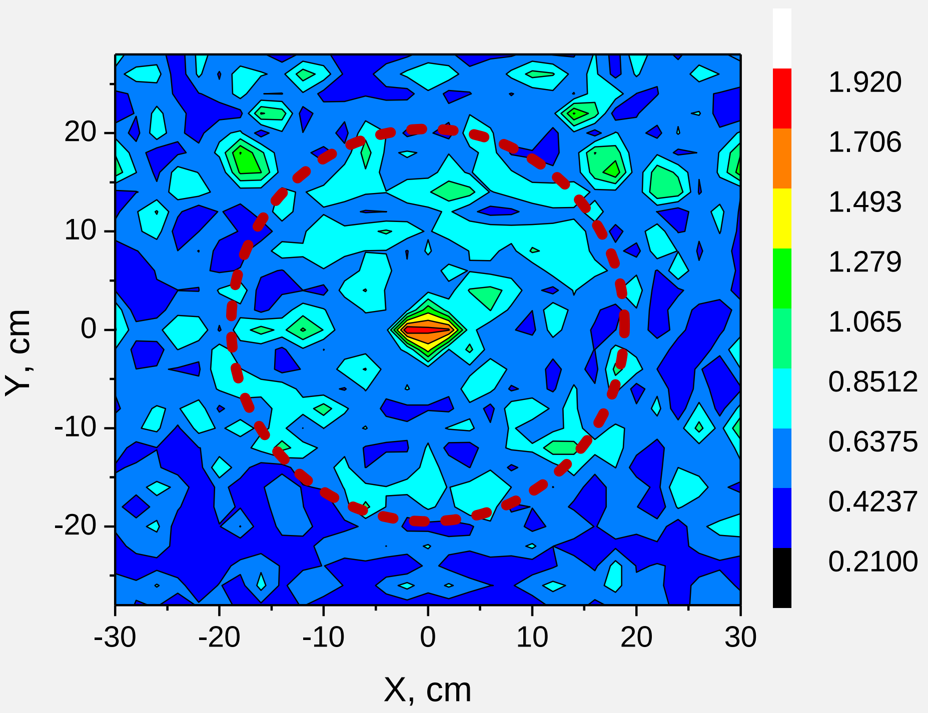
Diagram of experimental setup for hydrophone measurements in plexiglas box (the depth tangential to horn tip is defines z = 0; 1—Branson 902R Model transducer; 2—serial stepped ultrasonic horn; 3—Reson T4013 hydrophone; 4—water; 5—plexiglas box)

Large-Scale Evaluation



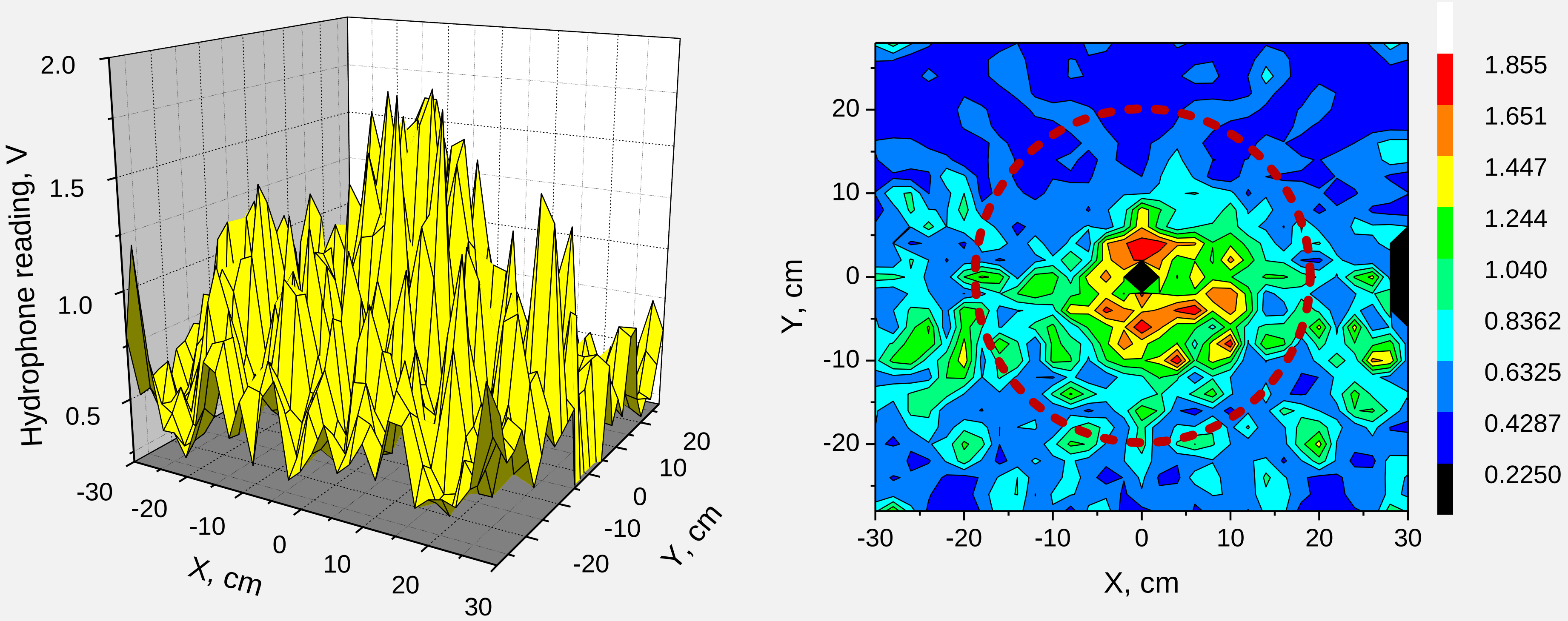
Large-Scale Application





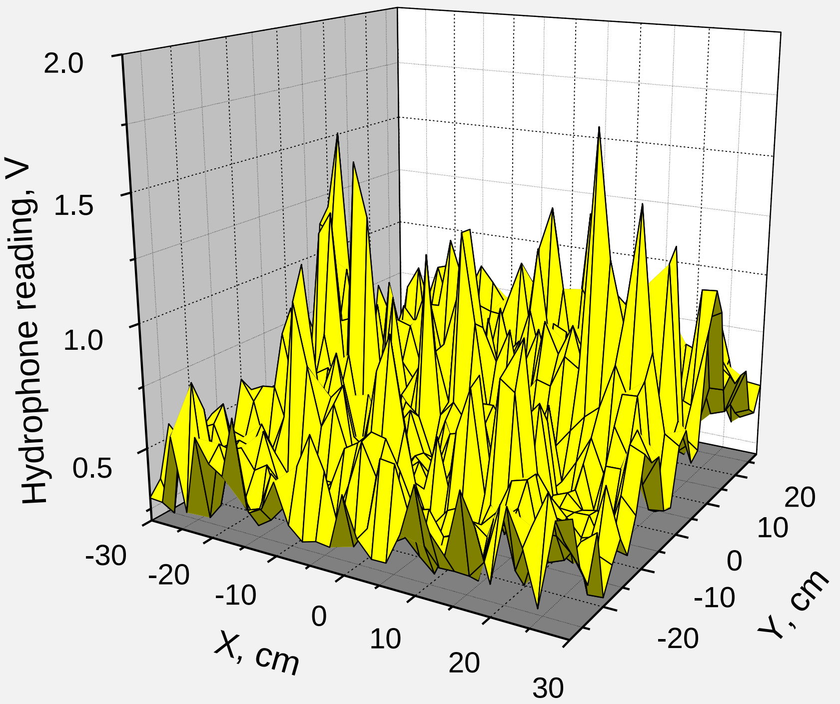
3D (left) and contour (right) mapping of hydrophone measurements in plexiglas tank (X–Y plane at **z = 0 cm**)

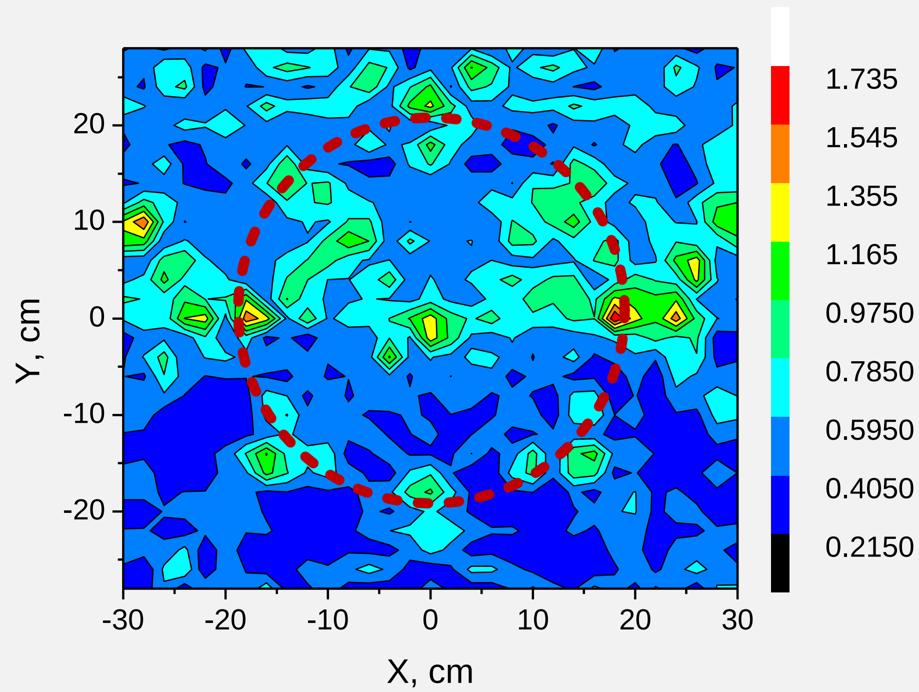
Large-Scale Application



3D (left) and contour (right) mapping of hydrophone measurements in plexiglas tank (X–Y plane at **z = +4 cm**)

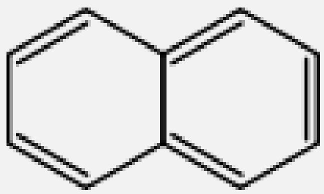
Large-Scale Application



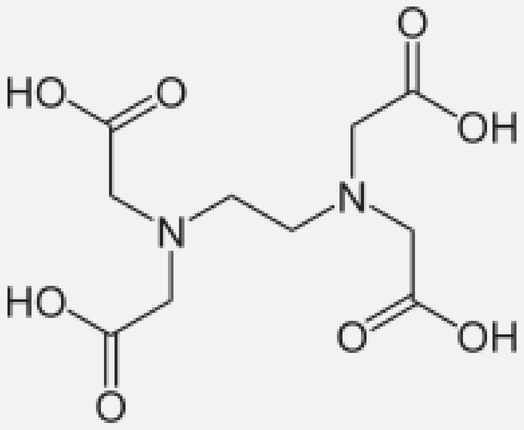


3D (left) and contour (right) mapping of hydrophone measurements in plexiglas tank
(X–Y plane at **z = –4 cm**)

Chemical Structure



Naphthalene



Ethylenediaminetetraacetic Acid (EDTA)

Schematic diagram of longitudinal vibration of single step horn and its equivalent circuits

$$\begin{cases} F_2 = \alpha_{21}\dot{\xi}_1 + \alpha_{22}F_1 \\ \dot{\xi}_2 = \alpha_{11}\dot{\xi}_1 + \alpha_{12}F_1 \end{cases}$$

$$\begin{bmatrix} \dot{\xi}_2 \\ F_2 \end{bmatrix} = \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{bmatrix} \begin{bmatrix} \dot{\xi}_2 \\ F_1 \end{bmatrix}$$

$$A_i = \begin{bmatrix} \alpha_{11}^i & \alpha_{12}^i \\ \alpha_{21}^i & \alpha_{22}^i \end{bmatrix} \qquad A_i = \begin{bmatrix} (\cos kl_i) & \dfrac{-j(\sin kl_i)}{\rho c S i} \\ -j\rho c S i(\sin kl_i) & (\cos kl_i) \end{bmatrix}$$

$$A = A_i A_{i-1} \cdots A_2 A_1 = \begin{bmatrix} \alpha_{11}^i & \alpha_{12}^i \\ \alpha_{21}^i & \alpha_{22}^i \end{bmatrix} \begin{bmatrix} \alpha_{11}^{i-1} & \alpha_{12}^{i-1} \\ \alpha_{21}^{i-1} & \alpha_{22}^{i-1} \end{bmatrix} \cdots \begin{bmatrix} \alpha_{11}^2 & \alpha_{12}^2 \\ \alpha_{21}^2 & \alpha_{22}^2 \end{bmatrix} \begin{bmatrix} \alpha_{11}^1 & \alpha_{12}^1 \\ \alpha_{21}^1 & \alpha_{22}^1 \end{bmatrix}$$

$$A = \begin{bmatrix} (\cos kl_8) & \dfrac{-j(\sin kl_8)}{\rho c S i} \\ -j\rho c S i(\sin kl_8) & (\cos kl_8) \end{bmatrix} \cdots \begin{bmatrix} (\cos kl_1) & \dfrac{-j(\sin kl_1)}{\rho c S i} \\ -j\rho c S i(\sin kl_1) & (\cos kl_1) \end{bmatrix}$$

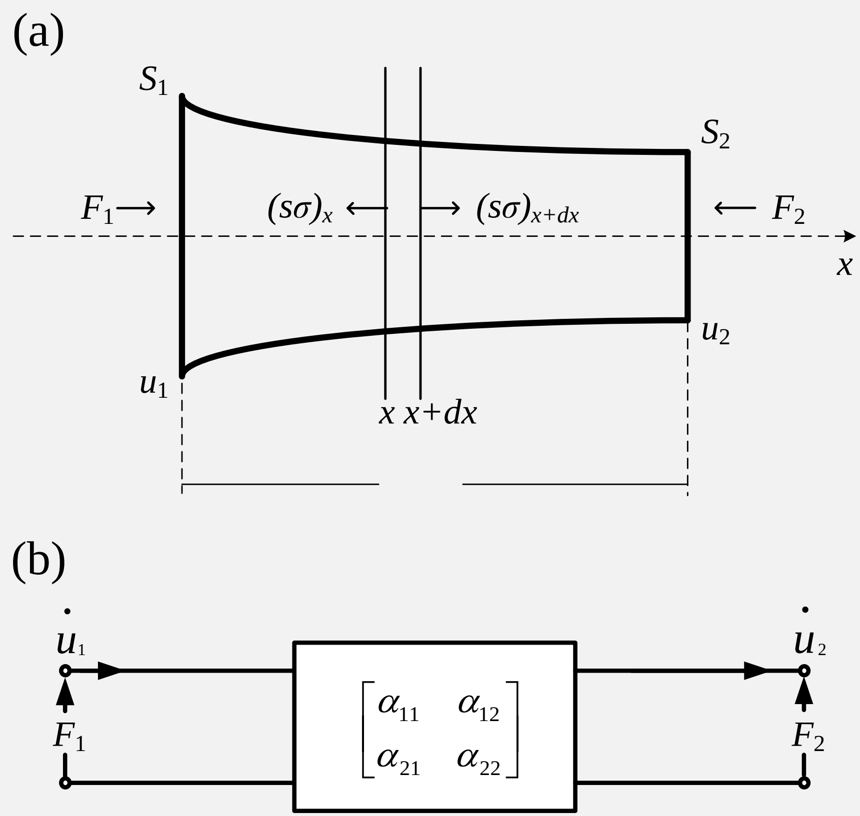
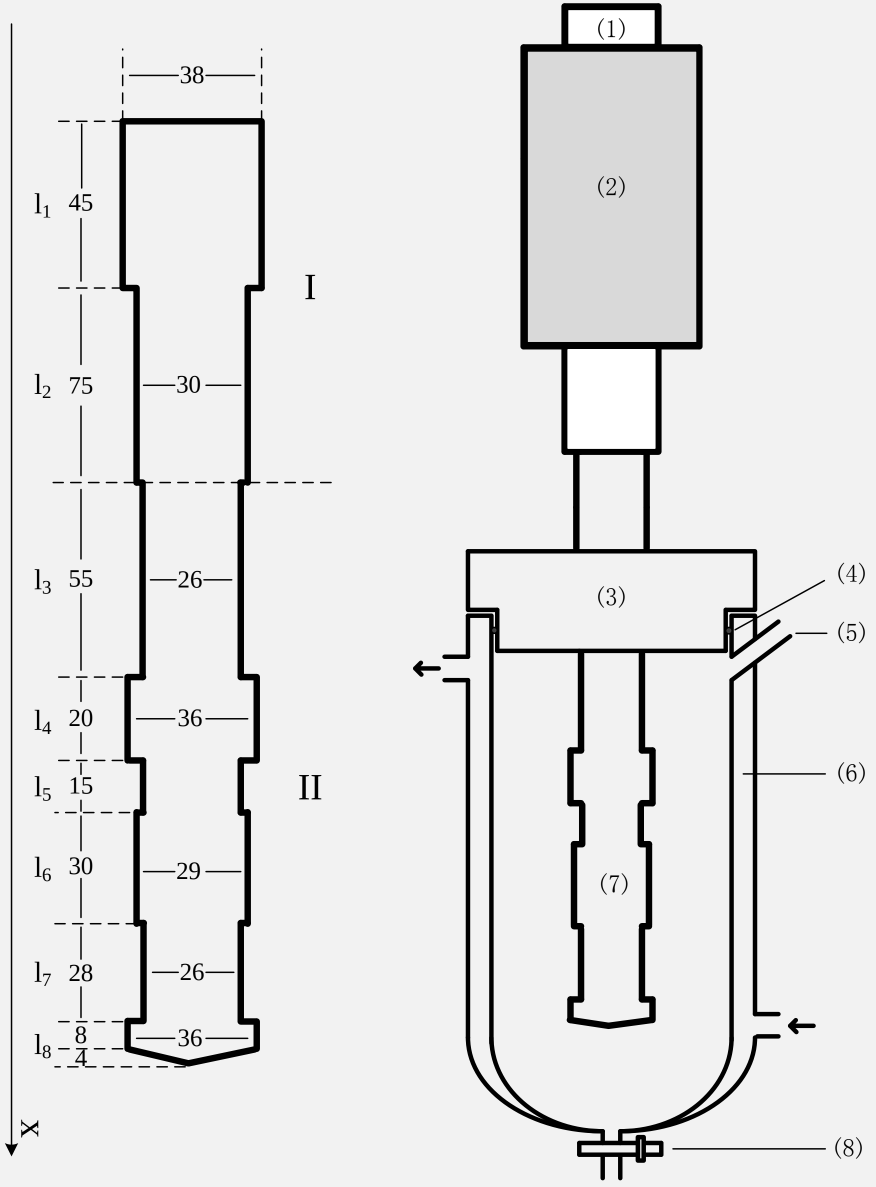


Diagram of experimental set-up



(a) (b)