MODELLING DISSOLVED OXYGEN CONTENT IN WATER FOR ULTRASOUND POWER MEASUREMENTS

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Ultrasound therapy devices are widely used to deliver prescribed doses to patients with a reasonable degree of accuracy. Excessive exposures either lead to unnecessary risk or fail to achieve clinical benefit. Regulations were then established to improve the quality of medical service and to protect patients around the world, for example, Safety Codes 23 and 24 in Canada. For these reasons, a primary ultrasound measurement system was developed at the National Research Council Canada for measuring the total ultrasonic power generated by an ultrasound transducer. The system was implemented according to the international standard, IEC 61161:1998. The second edition of IEC 61161 has been published since 2006. Edition 2 (2006) retains the same basic structure as Edition 1 (1998). However, more restrictive requirements for measuring conditions are put in place. A noticeable change is that when using a radiation force balance for determining output ultrasonic powers, only degassed water shall be used and the amount of dissolved oxygen in the water shall be less than 4 mg/l during all measurements. A simply solution for meeting this requirement is to deploy a dissolved oxygen (DO) meter. This will, however, create unpredictable ultrasound scattering in water tank. It is not a good choice for an existing system that has been optimized for minimum multipath effect using ray tracing technique. In this paper, a modelling method for the determination of dissolved oxygen in water was proposed as the solution. The dissolved oxygen contents were calculated by solving a diffusion equation with given initial and boundary conditions. To validate the model the predicted values were compared with those obtained by experiments.

Keywords: ultrasound power measurements, dissolved oxygen contents

1. Introduction

Ultrasound therapy devices are widely used to deliver prescribed doses to patients with a reasonable degree of accuracy. Excessive exposures either lead to unnecessary risk or fail to achieve clinical benefit. Regulations were then established to improve the quality of medical service and to protect patients around the world, for example, Safety Codes 23 and 24 in Canada [1, 2]. For these reasons, a primary ultrasound measurement system was developed at the National Research Council Canada (NRC) for measuring the total ultrasonic power generated by an ultrasound transducer [3]. The system was implemented according to the international standard, IEC 61161:1998 [4]. The second edition of IEC 61161 has been published since 2006 [5]. (Although there is a latest version of IEC 61161 published in 2013, but the decision of implementing according to IEC 61161-2006 is more managerial than technical.) Edition 2 (2006) retains the same basic structure as Edition 1
However, more restrictive requirements for measuring conditions are put in place. A noticeable change is that when using a radiation force balance for determining output ultrasonic powers, only degassed water shall be used and the amount of dissolved oxygen in the water shall be less than 4 mg/l during the period all measurements were made. A simply solution for meeting this requirement is to deploy a dissolved oxygen (DO) meter. This will, however, create unpredictable ultrasound scattering in water tank as the probe of the DO meter has an irregular shape and is compatible in size to the ultrasound wavelength. It is not a good choice for an existing system that has been optimized for minimum multipath effect using ray-tracing technique [6]. For NRC’s system, it is compliant with the requirements of ISO/IEC 17025 [7]. When some changes are made in the system, the influence of such changes should be documented and a new validation should be carried out. The validation results must be peer-reviewed on-site, regionally and inter-regionally and then approved by International Bureau of Weights and Measures. Furthermore, the DO meter cannot measure the dissolved oxygen contents in the water column under (or above depending on the transducer mounting) the transducer. It is the dissolved oxygen in this column that matters as cavitation occurs there first. In this paper, a modelling method for the determination of dissolved oxygen in water was proposed as the solution. The dissolved oxygen contents were calculated by solving a diffusion equation with given initial and boundary conditions. To validate the model the predicted values were compared with those obtained by experiments.

2. Modelling

If the exchange of oxygen across air-water interface is known, the dissolved oxygen in a water tank can be modelled as a diffusion process. Usually, the diffusion process is modelled by Fick’s law where the concentration gradient is the driving force for the diffusion. The diffusion in water is based on the hypothesis that the rate of transfer of diffusing oxygen through unit area of a section is proportional to the concentration gradient measured normal to the section. If the diffusion coefficient $D$ is constant, the concentration of diffusing oxygen $C$ is given by [8]

$$\frac{\partial C}{\partial t} = D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right)$$  \hspace{1cm} (1)

where $x$, $y$, and $z$ are the space coordinates and $t$ is the time.

For diffusion in a cylinder (water tank), by transformation of coordinates the above equation becomes

$$\frac{\partial C}{\partial t} = D \frac{1}{r} \left[ \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{1}{r} \frac{\partial C}{\partial \theta} \right) + \frac{\partial}{\partial z} \left( r \frac{\partial C}{\partial z} \right) \right]$$ \hspace{1cm} (2)

where $r$, $\theta$, and $z$ are the cylindrical coordinates.

A standard method to obtain a solution of a partial differential equation is assuming that the variables are separable. Thus, a solution of Eq. (2) may be written as

$$C = DR(r)\theta(\theta)Z(z)T(t)$$  \hspace{1cm} (3)

where $R$, $Z$, and $T$ are functions of $r$, $z$, and $t$ respectively. Assume the water tank is cylindrical symmetry. Thus, $\theta$ is not a function of $\theta$, but a constant.

In the following considerations, the diffusion process is decomposed into diffusion along $z$-axis and $r$-axis. That is, to decompose the diffusion into two parts acting in orthogonal directions.

2.1 Diffusion in $r$-direction

Diffusion in $r$-direction is governed by the diffusion equation

$$\frac{\partial C}{\partial t} = D \frac{1}{r} \left[ \frac{\partial}{\partial r} \left( r \frac{\partial C}{\partial r} \right) \right]$$ \hspace{1cm} (4)
with the following boundary and initial conditions for a water tank with a radius of \( a \)
\[
C = 0, \quad \text{for } r = a, \ t \geq 0 \tag{5}
\]
\[
C = C_0, \quad \text{for } 0 < r < a, \ t = 0 \tag{6}
\]
if the surface \( r = a \) (on tank side wall) is maintained at zero concentration and the initial concentration distribution is \( C_0 \), a constant.

The solution of the diffusion equation (Eq. 4) satisfying the boundary and initial conditions (Eqs. 5 and 6) is
\[
C = \frac{2}{a^2} \sum_{n=1}^{\infty} J_0(r \alpha_n) \int_0^J C_0 r J_0(r \alpha_n) \ dr \ e^{-D \alpha_n^2 t} \tag{7}
\]
where \( J_0(\alpha) \) is the Bessel function of the first kind of order zero and \( \alpha_n \) is determined from the root of \( J_0(a \alpha_n) = 0 \).

### 2.2 Diffusion in \( z \)-direction

The governing equation for diffusion in \( z \)-direction is
\[
\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} \tag{8}
\]
with the following boundary and initial conditions for a water tank with a depth of \( h \)
\[
C = 0, \quad \text{for } z = 0, \ t \geq 0 \quad \text{and} \quad C = C_1, \quad \text{for } z = h, \ t \geq 0 \tag{9}
\]
\[
C = C_0, \quad \text{for } 0 < z < h, \ t = 0 \tag{10}
\]
if the surface \( z = 0 \) (on tank bottom wall) is maintained at zero concentration and the initial concentration distribution is \( C_0 \), a constant.

The general solution of the diffusion equation (Eq. 8) satisfying the boundary conditions (Eq. 9) is
\[
C = \frac{C_1}{h} z + \sum_{n=1}^{\infty} A_n \sin(\beta_n z) \ e^{-D \beta_n^2 t} \tag{11}
\]
with \( \beta_n = n \pi / h \).

The coefficients \( A_n \) can be determined by applying the initial condition (Eq. 10). That is,
\[
C_0 = \frac{C_1}{h} z + \sum_{n=1}^{\infty} A_n \sin(\beta_n z) \tag{12}
\]
Multiplying both sides of the above equation by \( \sin(m \pi / h) \), where \( m \) is an integer, and integrating both sides of the resulting equation from 0 to \( h \) gives the following result for the coefficients \( A_n \):
\[
A_n = \begin{cases} 
\frac{2C_1}{n \pi} & \text{if } n = 2k \\
\frac{4C_0 - 2C_1}{n \pi} & \text{if } n = 2k + 1
\end{cases} \tag{13}
\]
where \( k \) is an integer.

### 2.3 Oxygen transfer across air–water interface

Oxygen transfer across an air–water interface has been studied extensively for various environmental conditions. The film theory is one of the two analytical approaches commonly used to study the absorption of gases into water [9]. The so-called "film" is a thin region in the water immediately
below the air-water interface. The film has little resistance for oxygen to transfer through. The time required for a newly created water surface (after water poured in container) to become fully saturated is about $10^{-7}$ sec [10]. Therefore, the dissolved oxygen at the water surface is the maximum dissolved oxygen concentration in water, or the oxygen solubility in water. Solubility of oxygen in freshwater at various temperatures and pressure can be found from Table 6.2-6 in [11]. The oxygen solubility at a given temperature and pressure is the boundary condition for the concentration $c_1$ at $z = h$.

### 2.4 Diffusion coefficient

Calculating the diffusion coefficient in liquids often uses a correlation developed by Wilke and Chang, which is based on the Stokes-Einstein equation [12]. The equation is usually accurate to 10% for dilute solutions of nondissociating solutes [13]. There are a number of experimental studies [14-22] and reviews [23, 24] of oxygen diffusion in liquids, including water in particular. All of the results at room temperature tend to cluster around $2 \times 10^{-5}$ cm$^2$/s, but with a great deal of scatter [20, 23].

Han and Bartels determined the diffusion coefficient of oxygen in water as a function of temperature from −0.5 to 95 °C, using the Taylor dispersion technique with optical absorbance detection at 200 nm [25]. They found significant deviation from Stokes-Einstein behavior over this temperature range. The measured diffusion coefficients have moderate precision and accuracy, typically better than 2%. A practical interpolation formula for the water solvent is given by

$$\log_{10} \left( \frac{D}{cm^2 \cdot s^{-1}} \right) = -4.410 + 773.8/T - (506.4/T)^2$$  \hspace{1cm} (14)

where $T$ is the absolute temperature in kelvin.

To obtain the interpolation formula for laboratory room temperature from 20 to 23 °C, the measured data were refitted for new coefficients with a polynomial of order 3. The revised interpolation formula is:

$$\frac{D}{cm^2 \cdot s^{-1}} = -42.4792 + 6.9292 \cdot T - 0.3563 \cdot T^2 + 0.0060 \cdot T^3$$  \hspace{1cm} (15)

where $T$ is the room temperature in Celsius. The formula has an expanded uncertainty of better than 2.3%.

### 3. Experimental verification

#### 3.1 Experiment setup

The apparatus used for this study is shown in Figure 1. A commercial optical DO meter (ProODO from YSI Inc.) was modified by removal of the protection grid. The optical technique used by the DO meter does not require the stirring of water. Therefore, the diffusion process is not disturbed. A thermometer (F250 from Automatic Systems Laboratories Inc.) was introduced to monitor the temperature to ensure the diffusion coefficient of oxygen is nearly constant during the diffusion process. A vertical and horizontal translation stage was used for proper positioning of the DO probe. Screen doors were installed to block the air flow from heating, ventilation and air conditioning (HVAC) system. A small heat source (a low watt lamp) was used to compensate the cooling of water due to evaporation. Two water tanks were tried in the study. One has a diameter of 12.7 cm and a depth of 13.5 cm. The other has a diameter of 29.8 cm and a depth of 29.2 cm. The apparatus and supporting structure are placed of a granite table. A tuned mass damping technology is used in order to reduce the dynamic response of the structure. It is tuned to a particular structural frequency so that when the table resonance is excited, the damper will resonate out of phase with the structural motion of the structure. Vibration energy is then dissipated by the damper inertia force acting on the structure so that the ground vibration has insignificant effect on the diffusion process under investigation.
3.2 Measurement Results

![Photo of the apparatus used in the study.](image)

Figure 1: Photo of the apparatus used in the study.

![A typical set of measurements.](image)

Figure 2: A typical set of measurements.

Measurements were performed during 18 working days with the focus on the dissolved oxygen contents in the small water tank, as cavitation is easier to occur in small confined space. The dis-
solved oxygen amount was measured at the center of the water tank with a depth of 10 mm from the water surface. This is the position of the active surface of an ultrasound transducer where the cavitation occurs first. A typical set of measurements without water temperature compensation is shown in Figure 2.

The measurement results are consistent over the time. To further improve the experiment a non-stirring DO probe and a heat source were applied. With a feedback control unit for the heat source the water temperature can be controlled within ± 0.5 °C.

4. Application

An immediate application of the modelling is to find the amount of dissolved oxygen in the water at a given location and time by using the solution of Eq. (1). As the time increases to certain point, the amount of dissolved oxygen at some location(s) may exceed a limit. The elapsed time, or the difference between the beginning and this point, is the operation time window for ultrasound power measurements.

4.1 Maximum dissolved oxygen amount

The locations of the maxima and minima dissolved oxygen amount in the water can be found by the zeros of the solution's derivative of the first order. A global maximum can then be found by comparing the maxima. The following Bessel function properties are useful in the derivation:

\[ J_{-n}(x) = (-1)^n J_n(x) \] (16)

\[ \frac{d}{dx} J_v(x) = \frac{1}{2} (J_{v-1}(x) - J_{v+1}(x)) \] (17)

Alternatively, one may spatially sample the locations in the water and calculate the dissolved oxygen amount at these locations to find a maximum. This approach, however, introduces additional uncertainty contribution due to sampling error. Such a contribution is very difficult to estimate. Therefore, this approach is not recommended.

4.2 Uncertainty of the amount of dissolved oxygen

The solution obtained in Section 2 for Eq. (1) is the expression for calculating the amount of dissolved oxygen in the water. This expression has three measured parameters: \( C_0 \), \( C_1 \), and \( D \) and it can be denoted as \( f(C_0, C_1, D) \). Uncertainty propagation occurs when mathematical operations are performed on measured quantities. The mathematical operations \( f(C_0, C_1, D) \) are performed on the measured quantities \( C_0 \), \( C_1 \), and \( D \) with the uncertainties of \( \delta C_0 \), \( \delta C_1 \) and \( \delta D \), respectively, to obtain the amount of dissolved oxygen \( C \). This results in the uncertainty propagation from \( \delta C_0 \), \( \delta C_1 \) and \( \delta D \) to \( \Delta C \), the uncertainty of the calculated \( C \). For the case of this application, all measured quantities \( (C_0, C_1, and D) \) are independent. The combined standard uncertainty \( \Delta C \) is then the positive square root of the combined variance \( \Delta C^2 \) that is given by [26]

\[ \Delta C^2 = \left( \frac{\partial f}{\partial C_0} \right)^2 \text{E}[\delta C_0^2] + \left( \frac{\partial f}{\partial C_1} \right)^2 \text{E}[\delta C_1^2] + \left( \frac{\partial f}{\partial D} \right)^2 \text{E}[\delta D^2] \] (18)

The amount of dissolved oxygen \( C \) and its associated uncertainty \( \Delta C \) only need to be calculated at the global maximum found in Section 4.1 as cavitation occurs there first. With the known \( C \) and \( \Delta C \), one can determine whether the amount of dissolved oxygen in the water at a time instance \( t \) conforms the requirement of IEC 61161:2006 according to the Joint Committee for Guides in Metrology document, JCGM 106:2012, Evaluation of measurement data – The role of measurement uncertainty in conformity assessment.
4.3 Upper limit

This modelling method assumes that the water surface is exposed to air all the time. That is, oxygen transfers across the entire air–water interface. In practice, a small central part of the water surface is covered by ultrasound transducer. At the surface of transducer, there is no dissolved oxygen (similar to those at the wall of water tank). This results in less oxygen transferred across the air–water interface compared with that (no transducer covering) used in the modelling. Thus, the calculated dissolved oxygen amount using this model is only an upper limit. Furthermore, vaporization occurs on the water surface. As the faster-moving molecules escape, the remaining molecules have lower average kinetic energy, and the temperature of the water decreases. This results in a slower diffusion process as the diffusion coefficient decreases with the decrease of the water temperature and ensures that the actual dissolved oxygen amount does not exceed the calculated upper limit.

5. Discussions

With Eq. (18), the confidence intervals of the calculated dissolved oxygen amount at the global maximum over the time can be found. These intervals are then compared with the confidence intervals of the measured dissolved oxygen amount using the DO meter. If two curves have non-overlapping confidence intervals, they are necessarily significantly different but if they have overlapping confidence intervals, it is not necessarily true that they are not significantly different. One has to calculate the test statistic for the difference between two means based on the square root of the sum of squares of the standard errors [27]. The t-statistic results show that the calculated dissolved oxygen amount is not statistically different from that of measured.

Some limitations of the modelling method were discussed in Section 4.3. These limitations can be overcome by solving the diffusion equation numerically instead of aiming a closed-form solution. The detailed work, however, is beyond the scope of this paper.

6. Conclusions

This work has contributed two advances to monitoring the amount of dissolved oxygen in the water during the period of all ultrasound power measurements made: 1) an expression for calculating the dissolved oxygen amount in water for given boundary and initial conditions, and 2) an application demonstrating how to use the expression to ensure the compliance of IEC 61161:2006. With these advances, an existing system can comply with the dissolved oxygen content requirement of IEC 61161:2006 without any system modification. Thus, costly system validations can be avoided.

REFERENCES


