NONLINEAR ACOUSTIC BEAM PROPAGATION MODELING IN DISSIPATIVE MEDIA

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ABSTRACT

Accurate simulation of an intensive ultrasound beam requires taking nonlinear propagation effects into account. A notable example in the field of biomedical ultrasound where the effect of nonlinearity may play a significant role is the high intensity focused ultrasound (HIFU) as a non-invasive energy-based treatment modality. In this work, a 3D numerical model to simulate nonlinear propagation of continuous wave ultrasound beams in dissipative homogeneous tissue-like media is presented. The model implements a second-order operator splitting method in which the effects of diffraction, nonlinearity and attenuation are propagated over incremental steps. The model makes use of an arbitrary 3D source geometry definition method and a non-axi-symmetric propagation scheme, which leads to a 3D solution to the resulting nonlinear ultrasound field. This work builds on methods developed by Tavakkoli et al. (1998) and Zemp et al. (2003) and offers an efficient way to calculate nonlinear field of continuous wave ultrasound sources. The proposed model is a particularly useful computational tool in carrying out simulations of high intensity focused ultrasound beams in soft tissue where the effects of nonlinearity, diffraction, and attenuation are important. The model was validated through comparisons with other established linear and nonlinear numerical models as well as published experimental data.

1. Introduction

Propagation of ultrasound is inherently a nonlinear process (Hamilton and Blackstock 1998). Nonlinear effects of ultrasound propagation such as waveform distortion and generation of harmonics can be observed in many biomedical applications of ultrasound (Carstensen and Bacon 1998). Two notable examples where the effects of nonlinear beam propagation play major roles in bioeffects of ultrasound are high intensity focused ultrasound (HIFU) and lithotripsy where intensive and focused ultrasound beams are used for various tissue treatments. Linear equations can be obtained assuming small signal approximations around equilibrium values of pressure and density. As the acoustic pressure and intensity levels are increased within the medium, more deviation from a linear model is expected.
Method of fractional steps

In our model the field is calculated plane by plane in a marching scheme. Consider a partial differential equation in the form of an evolution equation as:

$$\frac{\partial f}{\partial z} = L_{\text{par}} f$$  

(1)

where \( f \) is a function of \( x,y,z,t \) and \( L_{\text{par}} f \) is an operator which only acts on \( x,y,t \) dimensions. The term \( \frac{\partial f}{\partial z} \) on the left side of the equation enables plane by plane calculations of the function \( f \) in incremental steps along the \( z \) axis provided the values of \( f \) is known on an initial plane (e.g. at \( z=0 \)). This method is commonly referred to as method of fractional-steps (Ames 1992). The KZK equation can also be written in a form similar to Eq. (1) as shown below (Cobbold 2007, pp.254):

$$\frac{\partial p}{\partial z} = \frac{c_{\text{p}}}{2} \int \nabla^2 d\tau + \frac{1}{2c_{\text{p}}\rho_{\text{p}}} \left[ \left( \mu_\text{b} + \frac{4}{3} \mu_\text{c} \right) \frac{\partial^2 p}{\partial \tau^2} + \beta \frac{\partial p}{\partial \tau} \right]$$  

(2)

The first term in the right hand side of Eq. (2) represents diffraction, the second term accounts for attenuation and the third term appears because of nonlinearity. In our model, however, as will be explained in the next section, the diffraction operator is different from what is used in the KZK equation.

As it was suggested by Tavakkoli et al. (1998), the right hand side of Eq. (2) can be divided into three parts and rewritten in a general evolution equation form as below:

$$\frac{\partial p}{\partial z} = L_{\text{d}} p + L_{\text{a}} p + L_{\text{NL}} p$$  

(3)

where \( L_{\text{d}} p = \frac{c_{\text{p}}}{2} \int \nabla^2 d\tau \) is the diffraction operator,

$$L_{\text{a}} p = \frac{1}{2c_{\text{p}}\rho_{\text{p}}} \left( \mu_\text{b} + \frac{4}{3} \mu_\text{c} \right) \frac{\partial^2 p}{\partial \tau^2}$$  

is the attenuation operator and \( L_{\text{NL}} p = \frac{1}{2c_{\text{p}}\rho_{\text{p}}} \beta \frac{\partial p^2}{\partial \tau} \) represents the operator of nonlinearity. Eq. (3) demonstrates how operators of diffraction, nonlinearity and attenuation can be applied independently and then the results are added together. This is referred to as operator splitting method and has been schematically illustrated in Fig. 1(a). In our model, however, we have made use of a second-order operator-splitting method which follows a certain propagation scheme as illustrated in Fig. 1(b). Using the second-order operator splitting method would enable using larger propagation steps while maintaining the same degree of accuracy (Tavakkoli et al. 1998).

Diffraction operator

Using the second-order operator splitting method, the first step in propagating the field from the initial plane involves a half step diffractive propagation as shown in Fig. 1(b). The main difference between this method and implementation of the KZK equation lies in the diffraction step. The diffraction term of \( \frac{c_{\text{p}}}{2} \int \nabla^2 d\tau \) in the right hand side of the KZK Eq. (2) is only an approximation based on paraxial assumption. A more general term for diffraction should account for pressure distribution over the entire propagation plane and not only for the transversal Laplacian of pressure at each point. In this method the diffraction term in the KZK equation is replaced by a full diffraction solution. This is achieved by an angular spectrum approach which enables plane to plane diffractive propagation. If two planes are perpendicular to the \( z \) axis and \( \Delta z \) is the distance between them, we have (Cobbold 2007 pp.125, Zemp et al. 2003):

$$s(x,y,z+\Delta z) = \frac{\chi_{\text{NL}}}{\chi_{\text{NL}}} \chi_{\text{NL}} \left[ s(x,y,z) \right] \times H(k_{\text{p}}, k_{\text{e}}, \Delta z)$$  

(4)

where the transfer function \( H(k_{\text{p}}, k_{\text{e}}, \Delta z) = e^{i c_{\text{p}} \left( k_{\text{p}} \cdot \Delta z \right) \left( -\text{c}_{\text{p}} \Delta z \right)} \), \( k = 2\pi(nf_0)/c_{\text{g}} \) and \( n \) is the harmonic number. The term \( s(x,y,z) \) in Eq. (4) could be any field parameter such as pressure, normal particle velocity or velocity potential. In our model, we choose to propagate the normal particle velocity (i.e. \( s(x,y,z) = v_{\text{n}}(x,y,z) \)), since in our model the
nolinearity and attenuation operator acts on the normal particle velocity as discussed below.

![Figure 1](image-url)

**Figure 1.** Operator splitting methods. (a) First order, and (b) second order.

**Nonlinearity and attenuation operators**

After finishing with the diffractive sub-step, the results are converted to the spatial domain and a nonlinearity and attenuation sub-step is subsequently followed as shown in Fig. 1(b). Combined effects of nonlinearity and attenuation are applied in one step using the solution obtained by Harran and Cook (Harran and Cook 1983) for nonlinear propagation of progressive plane waves in lossy media. In this method a finite number of harmonics \(N\) is captured at each plane and normal particle velocity at \(z + \Delta z\) is obtained from the harmonic values of the preceding plane as below:

\[
v_n(z + \Delta z) = v_n(z) + \frac{2\pi \beta L}{2c} \Delta z \left( \sum_{i=1}^{N} v_{i,n} + \sum_{i=1}^{N} v_{i,n}' \right) - \alpha_n(\sigma) \cdot v_n \Delta z
\]

where \(n\) is the harmonic number. Eq. (5) has to be repeated \(N\) times to calculate all harmonics for each propagation step.

**3D source definition**

The first step in calculating the nonlinear acoustic field is to propagate the field from the surface of the transducer to a plane close-by which is called the initial plane. The reason behind this is that the method of fractional steps and the angular spectrum technique are both based on plane by plane propagation while the source geometry in general can presume any non-planar shape. The first part of the problem is to introduce a method to fully describe any source geometry and the second part is to introduce a method to capture the field of an arbitrarily shaped transducer. The first part is handled though introduction of an elements matrix and the second part is solved by using the Rayleigh diffraction integral on the surface of the source. To be able to define any source geometry and excitation, the source is broken into an array of small rectangular elements. The elements specifications (location and excitation) are then saved into a \(16 \times N\) matrix which we refer to as the Source Elements Matrix. \(N\) is the total number of small rectangular surface elements and 16 is the number of attributes required to fully describe a surface element (Mashouf 2009).

**Full diffraction solution**

Since our method accounts for full diffraction, it is desirable that the first propagation step would also include full diffraction calculation. Furthermore it is important to have the field calculated on the initial plane as accurate as possible in order to minimize the effect of error propagation due to plane by plane propagation scheme in the method of fractional steps. In light of this, the field on the initial plane is calculated using the Rayleigh diffraction formula which is a surface integral over the entire source area as shown in Fig. 2(a). Alternatively one can use a phase shift method to estimate the field on the initial plane based on the value of the closest surface element by applying phase and amplitude correction factors as shown in Fig. 2(b). This method has been widely used for simulations of a spherically concaved transducer (Averkiou and Hamilton 1995, Christopher and Parker 1991, Filonenko and Khokhlova 2001). Although it is computationally less intensive, this method is an approximate solution and could yield significant errors for highly focused sources (Mashouf 2009). This can be explained by noting that the field at any point on the initial plane is a sum of contributions of all surface elements and cannot be simply presented by a phase and/or amplitude correction to the corresponding value at the source surface. Once the geometry and excitation of the source are defined, the pressure is calculated at discrete points on the initial plane (e.g. point A in Fig. 2-a) by making use of the Rayleigh diffraction integral over the entire surface of the source as below (Ocheltree and Frizzell 1989):

\[
P_A = \frac{j \rho c s}{\lambda} \int \frac{V_n e^{-(\alpha + \beta) r}}{r} dS
\]

where \(r\) is the distance between the field point and an infinitesimal surface element, \(V_n\) is the normal velocity phasor at the element surface and \(dS\) is the area of the infinitesimal surface element.

Since in our model, the source is defined by a set of small rectangular elements, Eq. (6) is realized as below:

\[
P_A = j \rho c s \sum_{i=1}^{N} V_n e^{-(\alpha + \beta) r_i} \frac{w \cdot l}{r_i}
\]

where \(N\) is the total number of surface elements, \(r_i\) is the distance between the field point and the center of the \(i\)th surface element, and \(w\) and \(l\) are the width and the length of each surface element respectively.
Figure 2. Schematic demonstration of the ultrasound field calculation over an initial plane by (a) implementing the Rayleigh diffraction integral, (b) introducing phase/amplitude correction factors. In method (a) contributions of all surface elements are taken into account while in method (b) only the value of the closest horizontally located element is used to estimate the field by applying a complex correction factor ($C_1, C_2$).

Field propagation

Field propagation is done in incremental steps following a second-order operator splitting method as described earlier. The first step involves a half step diffusive propagation as illustrated in Fig. 1(b). Each harmonic is propagated separately by applying Eq. (4) as below:

$$\bar{\mathbf{v}}_{n+\frac{1}{2}}(x, y, z + (\Delta z/2)) = \mathbf{F}^{-1} \left[ \mathbf{F} \mathbf{v}_{n}(x, y, z) \cdot \mathbf{H}(k_x, k_y, (\Delta z/2)) \right]$$

where the transfer function $H(k_x, k_y, (\Delta z/2)) = e^{(ik_x x + ik_y y) \Delta z/2}$

and $\Delta z$ is the size of each propagation step. The 2D Fourier transform of normal particle velocity on the initial plane is can be obtained as (Mashouf 2009):

$$\mathbf{F} \mathbf{v}_{n}(x, y, z_0) = w^2 \text{sinc}(w k_x / 2\pi, w k_y / 2\pi) \cdot \sum_{i=1}^{N} \mathbf{v}_i e^{-j(k_x x_i + k_y y_i)}$$

where $N$ is the total number of the array elements. Accordingly the right hand side of Eq. (8) can be obtained by multiplying Eq. (9) to the transfer function $H$.

After finishing the diffraction substep, the result is converted back to spatial domain using inverse 2D Fourier transform and a nonlinear substep is subsequently followed as shown in Fig. 1(a). The process is then repeated to propagate the field along the $z$ direction.

Spatial sampling

Since performing the 2D inverse Fourier transform of Eq. (8) is analytically not possible, the right hand side of this equation is discretized along $k_x$ and $k_y$ dimensions and an inverse discrete Fourier transform is used instead. The sampling of $k_x$ and $k_y$ dimensions should be performed to capture the field variations adequately. If $\Delta x$ is the desired sampling interval on a propagation plane over the $x$ dimension, the maximum spatial frequency component of the 2D discrete Fourier transform of the field over the $k_y$ dimension is given by:

$$k_{y, max} = \frac{\pi}{\Delta x}$$

As mentioned before, the first propagation step involves a diffusive sub-step which is calculated as below (see Eqs. (8) and (9)):

$$\mathbf{v}_{n+\frac{1}{2}}(x, y, z_0 + (\Delta z/2)) = \mathbf{F}^{-1} \left[ \mathbf{F} \mathbf{v}_{n}(x, y, z) \cdot \sum_{i=1}^{N} \mathbf{v}_i e^{-j(k_x x_i + k_y y_i)} \cdot \mathbf{H}(k_x, k_y, (\Delta z/2)) \right]$$

Studying a $\text{sinc}(x)$ function shows that at around $x = 5$, its amplitude has already reduced to about 5% of the maximum. Hence, the values of $w k_x / 2\pi$ in Eq. (11) should extend beyond 5 in order for variations to be adequately captured. In other words:

$$\frac{w k_x}{2\pi} \geq 5$$

Substituting $k_{y, max}$ form Eq. (10) into Eq. (12), the following criteria for the sampling interval is obtained:

$$\Delta x \leq \frac{\pi}{10}$$

Similar criterion applies for sampling interval along $y$ direction. In other words the spatial sampling on the propagation plane should be at least ten times finer than that of the initial plane.

Enhanced pressure formulation

In the methodology described above, the values of normal particle velocity ($\mathbf{v}_n$) are calculated on each propagation plane. Other acoustic parameters such as pressure should be derived from the calculated values of normal particle velocity. A simple method to convert normal particle velocity to pressure, is through the linear impedance relation as below:

$$P(x, y) = \rho_0 c_0 \cdot V_z(x, y)$$

This formula, however, is only accurate for a plane wave travelling along the $z$ axis in an inviscid medium. As we will see later, Eq. (14) can be significantly in error in nonplanar fields. A more general formula which is valid in any field configuration (such as spherical, cylindrical or focused beams) is expressed as below (Liu and Waag 1997):
Eq. (15), however, includes a singularity in spatial frequency at a circle with radius of $k$ which is centered at origin and known as radiation circle. As a result, numerical methods to calculate the inverse Fourier transform of Eq. (15) may either fail or generate considerable amount of computational noise in the output. Eq. (15) assumes propagation in a lossless medium. In the presence of viscous loss, Eq. (15) takes the following form (see Mashouf (2009) for the full derivation):

$$P(x, y) = \mathcal{F}^{-1} \left\{ \mathcal{F}_2 \left\{ \left( \frac{\rho c k}{\sqrt{k^2 - (k_x^2 + k_y^2)} } \right) \right\} \right\}$$

Eq. (16)

where $k^2 = \frac{k^2}{1 - j(2a/k)}$. In a lossless medium, $k^2 = k^2$ and Eq. (16) reduces to Eq. (15) as expected. It is interesting to note that in the presence of viscous loss, the transfer function of Eq. (16) will no longer contain a singularity. Since in a physical medium there's always some loss, the problem of singularity can therefore be avoided by using Eq. (16).

It can be also shown that in case of a plane wave propagating in an inviscid medium Eq. (16) reduces to the impedance relation of Eq. (14) as expected. In a plane wave propagating along the $z$ direction, normal particle velocity phasor is a constant anywhere on a plane perpendicular to the $z$-axis. In other words $\nu_z(x, y) = \nu_z$, where $\nu_z$ is a constant.

As a result 2D Fourier transform of $\nu_z(x, y)$ is a Dirac impulse function as below:

$$P(x, y) = \mathcal{F}^{-1} \left\{ \mathcal{F}_2 \left\{ \delta(k_z, k_z) \right\} \right\}$$

or

$$P(x, y) = \mathcal{F}^{-1} \left\{ \mathcal{F}_2 \left\{ \delta(k_z, k_z) \right\} \right\}$$

Since in an inviscid medium $k = k$, Eq. (19) can be simplified further as below:

$$P(x, y) = \rho c \mathcal{F}^{-1} \left\{ \mathcal{F}_2 \left\{ \delta(k_z, k_z) \right\} \right\}$$

Conversely, the inverse 2D Fourier transform of a delta function is a constant in space. In other words:

$$P(x, y) = \mathcal{F}^{-1} \left\{ \mathcal{F}_2 \left\{ \delta(k_z, k_z) \right\} \right\} = \rho c \nu_z$$

which is the well-known impedance relation.

Eq. (16) enables conversion of particle velocity normal to a plane to the values for pressure on the same plane. Since in our method the values of normal particle velocity are only known over the extent of propagation planes, Eq. (16) serves as an ideal tool to accomplish conversion to the values of pressure.

We refer to pressure obtained using Eq. (16) as “enhanced pressure” formulation to make distinction from the impedance pressure formulation expressed by Eq. (14). In what follows we demonstrate how impedance pressure of Eq. (14) can be significantly in error in non-planar fields.

**Field of a concave spherical source**

Another example of a non-planar acoustic field is the field of a concave spherical source. It is important to investigate the degree of error in the plane wave approximation used in this geometry that is frequently used in many biomedical applications including HIFU. We study three transducers with different $F$ numbers to demonstrate how the source curvature affects the results. Focal distance of all transducers are equal (20mm) but they have different diameter of apertures as shown in Figs. 3(a). As a result, the associated $F$ numbers of the transducers will be 2 and 1. Figs. 3(b) and (c) display the lateral pressure profiles on the focal plane of each transducer. Each graph shows two pressure profiles which have been obtained using different methods namely the Rayleigh integral and the impedance formula. The Rayleigh integral was calculated using Eq. (7), and the linear impedance formula makes use of the plane wave approximation given by Eq. (14) as described before. As it can be seen in Fig. 3, the difference between the actual pressure and the plane wave approximation rises as the source curvature increases (or $F$ number decreases). This is expected as deviation from a plane wave is more pronounced in the case of a highly focused source versus a slightly focused source. The second point to note about pressure profiles presented in Fig. 3, is that the actual pressure is almost always higher than what is predicted by an impedance approximation. This can be explained by the fact that in the linear impedance formula, only the normal component of particle velocity ($v_n$) is used to estimate the pressure, but in general non-planar fields, lateral components of particle velocity (i.e. $v_x$, $v_y$) are also present and could have substantial amplitudes. Lateral components of the particle velocity would also contribute to creating a pressure build up.

### 3. Results

The KZK equation has been widely accepted as a gold-standard model to simulate nonlinear ultrasound propagation. In order to validate our methodology and test the performance of our model in nonlinear mode, we compared the results obtained using our model with published KZK simulations and experimental results. In their 1995 paper, Averkiou and Hamilton (Averkiou and Hamilton 1995) presented results of the KZK simulations for a concaved spherical source in water and compared them with experimental data. In order to do a comparative study, we implemented identical source and medium parameters (as used by Averkiou and Hamilton) in our model. The parameters used in this simulation include: Radius of...
Figure 3. (a) Concentric concaved spherical sources with different diameters of aperture (D) to study the effect of curvature in calculation of pressure. Higher values of D corresponds to higher degrees of focusing. Comparison of impedance pressure versus actual pressure at \( f_0 = 1 \) MHz on the focal plane of a (b) moderately focused and (c) a highly focused source.

Figure 4. Lateral pressure profiles at various axial locations (top panel: pre-focal, middle panel: focal plane, bottom panel: post-focal). Left column: Our model, Right column: Experiment (solid line) and KZK results (dotted line) by Averkiou and Hamilton, 1995.

4. Discussions and Conclusions

In this work a continuous wave nonlinear propagation model based on a second-order operator splitting method was presented. The model was made more versatile by introducing a 3D arbitrary source definition capability and by converting the values of normal particle velocity to pressure across the propagation plane using an enhanced formula in dissipative media. Using our numerical model, one can define any 3D source geometry. The amplitude and phase of the normal particle velocity can also be arbitrarily defined and varied across the source surface as appropriate. This would enable simulations of transducers of arbitrary geometries and excitations. The full diffraction and enhanced pressure formula enable calculation of the acoustic pressure in a given plane in terms of the normal particle velocity in the same plane (see Eq. (16)). We demonstrated that for a concave spherical source with dimensions and excitation frequencies around those of interest in biomedical ultrasound, the impedance relation based on the plane wave approximation yields substantially lower pressure values. A particular area of interest is the focal region of focused sources where a significant difference between the two methods is observed. The difference in predicted pressure leads to even more disparity in intensity values as the intensity is related to pressure by the power of two in nonlinear regime according to the approximate formula

\[
I_{\text{total}} = \sqrt{\sum_{n=1}^{N} \left| P_n \right|^2},
\]

which simply states that the total intensity in a nonlinear field is equal to...
the sum of intensities of each harmonic (Bailey et al. 2003). Moreover, since the intensity values are directly proportional to heat generation rate, according to the approximate formula \[ Q_{\text{total}} = \sum_{n=1}^{\infty} 2\pi r_n I_n \] (Bailey et al. 2003), this will in turn affect temperature predictions as well. Accurate temperature calculations are highly demanded in areas such as ultrasound hyperthermia and/or high intensity focused ultrasound (HIFU) where focused nonlinear ultrasound beams are used to induce controlled tissue temperature elevation. Through implementation of the enhanced pressure formula we managed to resolve the singularity issue in the transfer function of normal particle velocity to pressure by making use of \( k \) or a complex wave number. By using a complex wave number, the singularity in Eq. (15) is eliminated and calculating the inverse 2D Fourier transform becomes a well-posed problem. Alternatively this singularity can be avoided by implementing a narrow band-stop filter around the singularity. However the complex wave number method offers benefits in terms of calculation accuracy and efficiency over the filtering method (Mashouf 2009). We verified our results by comparison to simulation and experimental data available in the literature. A great agreement observed both in linear and nonlinear regimes. The next steps in this work include expansion of the current model to include temperature rise predictions, multilayer media and pulse mode propagation. The temperature simulations are carried out by calculating the heat deposition rate within the medium and coupling with an enhanced bio-heat transfer equation. Multilayer medium can be introduced into the model by changing the medium properties in each propagation step accordingly.

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