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## A Boundary Condition to the Khokhlov-Zabolotskaya Equation for Modeling Strongly Focused Nonlinear Ultrasound Fields

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Abstract. An equivalent source model was proposed as a boundary condition to the nonlinear parabolic Khokhlov-Zabolotskaya (KZ) equation to simulate high intensity focused ultrasound (HIFU) fields generated by medical ultrasound transducers with the shape of a spherical shell. The boundary condition was set in the initial plane; the aperture, the focal distance, and the initial pressure of the source were chosen based on the best match of the axial pressure amplitude and phase distributions in the Rayleigh integral analytic solution for a spherical transducer and the linear parabolic approximation solution for the equivalent source. Analytic expressions for the equivalent source parameters were derived. It was shown that the proposed approach allowed us to transfer the boundary condition from the spherical surface to the plane and to achieve a very good match between the linear field solutions of the parabolic and full diffraction models even for highly focused sources with *F*-number less than unity. The proposed method can be further used to expand the capabilities of the KZ nonlinear parabolic equation for efficient modeling of HIFU fields generated by strongly focused sources.

### **INTRODUCTION**

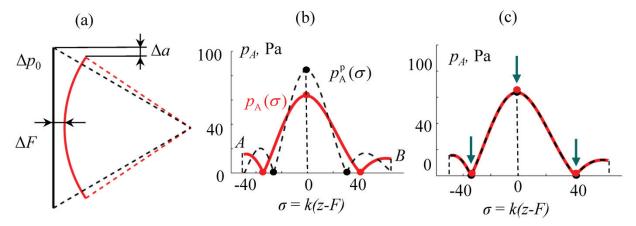
Nonlinear parabolic Khokhlov-Zabolotskaya (KZ) equation is a common model used for modeling high intensity focused fields generated by medical ultrasound transducers [1,2]. Simulations in water, where calibration of field parameters of such transducers is usually performed, have become an important metrological tool [3 - 5]. The equation itself includes parabolic approximation of the diffraction effects, which is valid for small angles of the beam focusing [6]. In addition, the boundary condition to the KZ model is set in the initial plane whereas most therapeutic sources typically have the shape of a spherical shell. The model therefore can be applied with reasonable accuracy for modeling weakly focused fields of ultrasound imaging transducers but there has been always a concern whether it can be used for strongly focused fields of the HIFU devices. Certain modifications to the KZ equation have been proposed including its modification for spheroidal coordinates to account for the converging angle of the beam or a wide-angle parabolic approximation of the diffraction effects [7,8]. Much less attention has been paid to the problem of an appropriate transfer of the boundary condition from the spherical surface of a real source to the plane for the KZ modeling. In most numerical studies the boundary condition was set in a plane crossing the transducer center as a piston source with the aperture and the uniform pressure amplitude being the same as for the real transducer, and the parabolic phase distribution that follows its focusing angle. For strongly focused beams, this direct approach results in significant underestimation of the focal pressure values and distortion of the spatial beam structure. However, several recent studies have shown that some change in the aperture and initial pressure in the parabolic boundary condition can be done, so that the results of simulations match the field measurements in the focal lobe even for transducers with F-number = 1, both for linear and nonlinear focusing conditions [3-5]. The goal of this study was to establish an improved equivalent source model for the KZ equation. Three parameters of the boundary condition, the aperture, the focal length, and the pressure amplitude, were varied to achieve the best match

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of the axial pressure amplitude and phase distributions of the linear parabolic approximation solution and the Rayleigh integral solution (Fig. 1). It was shown that the proposed approach allowed us to transfer the boundary condition from the spherical surface to the plane and to achieve a very good match between the linear field solutions of the parabolic and full diffraction models even for highly focused sources with *F*-number less than unity.

#### THEORETICAL METHOD

The idea of the method was to choose the location of the boundary condition plane, the source aperture, and initial pressure in the parabolic model (Fig. 1a) by minimizing the difference between the full diffraction and parabolic solutions for acoustic pressure amplitude on the axis of a linearly focused beam. Three unknown parameters of the equivalent source were found from a set of three equations that equalize the pressure amplitude at the focus  $p_A^p = p_A$  at  $\sigma = 0$ , and the position of two nulls of the focal diffraction lobe  $\sigma_1^p = \sigma_1$  and  $\sigma_2^p = \sigma_2$  (Fig. 1b,c); these three points of matching are indicated in Fig. 1b as black dots. Here, the upper index "p" corresponds to the parabolic model,  $\sigma = k(z-F)$  is the dimensionless coordinate along the transducer axis shifted to the focal point z = F, k is the wavenumber, F is the focal length.



**FIGURE 1.** Illustration of setting a boundary condition to the linear parabolic model for simulating focused ultrasound beams generated by single-element spherically-shaped transducers. (a) Variations in position ( $\Delta F$ ), aperture ( $\Delta a$ ), and pressure amplitude ( $\Delta p_0$ ) of the equivalent source given in the plane relative to the spherical source. (b) Pressure amplitude distributions calculated on the beam axis using a full diffraction  $p_A(\sigma)$  and parabolic  $p_A^p(\sigma)$  models: before matching, (c) after matching.

The Rayleigh integral solution of the full diffraction model for the axial pressure amplitude distribution  $p_A(\sigma)$  of a single-element source with a uniform pressure amplitude  $p_0$  at the surface of a spherical cup can be written in an analytic form [9]:

$$p_{\rm A}(\sigma) = \frac{2p_0}{|\sigma|} kF \left| \sin\left(\frac{\sigma + kF - kR_{\rm max}(\sigma, kF, \alpha)}{2}\right) \right|,\tag{1}$$

where  $R_{\text{max}}$  is the location  $\sigma$  on the axis and the edge of the transducer:  $kR_{\text{max}} = \sqrt{\sigma^2 + 2\sigma kF \sqrt{1 - (2\alpha)^{-2} + (kF)^2}}$ ,  $\alpha = F/2a$  is the *F*-number of the transducer, *a* is the aperture of the spherical source.

The axial solution to the parabolic model for the pressure amplitude distribution  $p_A^p(\sigma)$  of a single-element focused source with uniform pressure amplitude  $p_0^p$  at the plane surface can be also written in an analytic form as:

$$p_{\rm A}^{\rm p}(\sigma) = \frac{2p_0^{\rm p}}{|\sigma|} kF^{\rm p} \left| \sin\left(\frac{\sigma kF^{\rm p}}{16\alpha_{\rm p}^{\rm p} \left(\sigma + 2kF^{\rm p}\right)}\right) \right|.$$
<sup>(2)</sup>

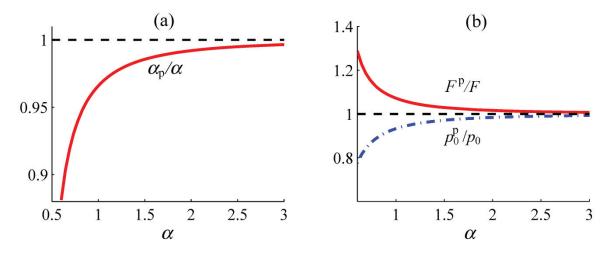
Geometrical parameters of the parabolic source,  $kF^p$ , and  $\alpha_p$  can be found by equalizing the position of two nulls around the focus in the solutions (1, 2), then the source amplitude  $p_0^p$  can be found by matching the focal pressures.

### **RESULTS**

The set of equations that determine the parameters of an equivalent source,  $kF^p$ ,  $\alpha_p$ , and  $p_0^p$ , can be solved analytically, but the solution is quite cumbersome. However, it can be simplified within the approximation of the large aperture and focal length compared to the wavelength, ka >> 1 and kF >> 1, which is almost always fulfilled for HIFU transducers. Using this approximation, the solutions can be written as follows:

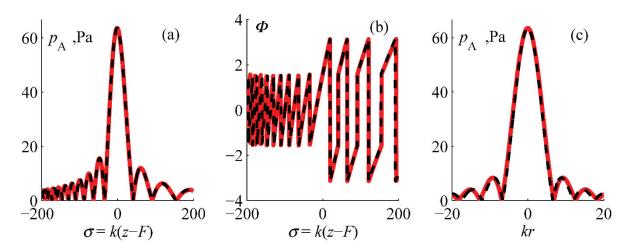
$$\begin{cases} \alpha_{\rm p} = 0.5 \cdot \left(2 - \sqrt{4 - 1/\alpha^2}\right)^{-1/2}, \\ kF^{\rm p} = \frac{kF \cdot 4\alpha^3 \left(\sqrt{\alpha} + 2\right)^2}{32\alpha^3 + \sqrt{4\alpha^2 - 1}\left(16\alpha^2 - 1\right) - 6\alpha}, \\ p_0^{\rm p} = p_0 F/F^{\rm p}. \end{cases}$$
(3)

Shown in Fig. 2 are the solutions (3) for the parameters  $kF^p$ ,  $\alpha_p$ , and  $p_0^p$  of the boundary condition to the parabolic model plotted as functions of the parameters of the spherical source. It is seen that modifications to all three parameters of the parabolic source depend only on the *F*-number =  $\alpha$  of the spherical source. According to these solutions, each parameter of the parabolic source can be obtained by scaling the corresponding parameter of the spherical source is always less focused, its focal length is longer, and the pressure amplitude is less than those of the spherical one.



**FIGURE 2.** Scaling curves for parabolic source parameters as compared to the spherical ones. Here  $\alpha$ , *F* and  $p_0$  are *F*-number, focal length, and pressure amplitude at the spherical source. Parameters with index "p" correspond to the parabolic model.

Although matching the fields was done for three points at the axis of the beam, good agreement was achieved within a large region around the focus even for a highly focused transducer with F-number = 0.9 (Fig. 3).



**FIGURE 3.** Axial (a,b) and radial (c) distributions of normalized pressure amplitude  $p_A$  (a) and axial phase  $\Phi$  (b) calculated using the full diffraction (solid line) and parabolic (dashed line) solutions for strongly focused HIFU transducer with 1 MHz frequency, a = 5 cm; F = 9 cm; and  $\alpha = 0.9$ . Parabolic equivalent source parameters:  $a_p = 5.7$  cm;  $F_p = 9.8$  cm;  $\alpha_p = 0.862$ .

#### CONCLUSION

A method to determine the aperture, focal length, and initial pressure amplitude of an equivalent piston source as a boundary condition to the KZ equation is proposed to simulate focused ultrasound beams generated by single element transducers with the shape of a spherical cup. Analytic solutions for the equivalent source parameters are obtained. Full diffraction and parabolic modeling results were compared for a linear beam focusing. It is shown that parabolic approximation with the equivalent source boundary condition can be successfully used for calculating fields from strongly focused HIFU transducers with *F*-number even less than unity. The proposed method can be applied for simulation of nonlinear beam focusing by scaling the initial pressure amplitude. It can be also used for modeling the field of complex transducers, such as multi-element arrays by matching the results of the KZ linear modeling to the beam scan measurements.

#### ACKNOWLEDGMENTS

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