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Camarena Femenia, F.; Adrián Martínez, S.; Jimenez, N.; Sánchez Morcillo, VJ. (2013). Nonlinear focal shift beyond the geometrical focus in moderately focused acoustic beams. *Journal of the Acoustical Society of America*. 134(2):1463-1472. doi:10.1121/1.4812865.



The final publication is available at

<http://dx.doi.org/10.1121/1.4812865>

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1 **Nonlinear focal shift beyond the geometrical focus in moderately focused acoustic**
2 **beams¹**

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9 Submitted June 2012

10 Focal shift in moderately focused beams

11
12 The phenomenon of the displacement of the position along the axis of the pressure,
13 intensity and radiation force maxima of focused acoustic beams under increasing
14 driving voltages (nonlinear focal shift) is studied for the case of a moderately focused
15 beam. The theoretical and experimental results show the existence of this shift along the
16 axis when the initial pressure in the transducer increases until the acoustic field reaches
17 the fully developed nonlinear regime of propagation. Experimental data show that at
18 high amplitudes and for moderately focusing the position of the on-axis pressure
19 maximum and radiation force maximum can surpass the geometrical focal length. On
20 the contrary, the on-axis pressure minimum approaches the transducer under increasing
21 driving voltages, increasing the distance between the positive and negative peak
22 pressure in the beam. These results are in agreement with numerical KZK model
23 predictions and the existed data of other authors, and can be explained according to the
24 effect of self-refraction characteristic of the nonlinear regime of propagation.

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27 PACS numbers: 43.25.Cb; 43.25.Jh; 43.25.Qp; 43.25.Zx

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¹ Special issue on Therapeutic Ultrasound

33 I. INTRODUCTION

34 The study of the acoustic field characteristics generated by focusing sources, both in
35 linear¹⁻³ and nonlinear⁴⁻⁸ regime, is a continuously developing field of research as sound
36 beams are relevant in most of the ultrasonic applications in medicine and industry.
37 Lucas and Muir³ studied the acoustic field generated by a focused source in linear
38 regime. This work showed that, due to the diffraction of the beam, the on-axis pressure
39 maximum position is not located at the geometrical focus, but closer to the source. The
40 distance between these two points is called the linear focal shift, and depends on the
41 source characteristics (aperture, geometrical focal length, and frequency) and the
42 medium properties⁹.

43 The nonlinear focal shift phenomenon, defined as the shift of the maximum pressure
44 (and also intensity and radiation force) position along the axis of focused acoustic
45 beams under increasing driving voltages, has also been discussed and interpreted in
46 previous works. In 1980 Bakhvalov et al.¹⁰ predicted a shift in the position of the on-
47 axis pressure maximum in unfocused beams where a migration of the location of the
48 maximum was shown, first away from, and then towards the transducer, as the exciting
49 voltage of the source was increased. Duck and Starritt¹¹ (1986) studied this phenomenon
50 in slightly focused sources as those used in commercial medical pulse-echo equipments,
51 showing that the nonlinear focal shift exists for on-axis maximum and minimum
52 pressure, with different behaviour. Averkiou and Hamilton¹² (1997) observed this
53 phenomenon experimentally in a moderately focused piston (linear gain $G=p/p_0=10.36$;
54 where p is the value of the pressure in the geometrical focus and p_0 the pressure at the
55 surface of the transducer). The nonlinear focal shift phenomenon was reported by
56 Makov et al.¹³ in low gain transducers, and discussed it in terms of the harmonics
57 nonlinearly generated during the propagation of a finite amplitude wave. They provided
58 also experimental evidence of the nonlinear shift in slightly focused transducers ($G=4$).
59 Recently, Bessonova et al.¹⁴ reported a numerical study where the nonlinear focal shift
60 is shown for a moderately focused piston ($G=10$) in a range of intensity covering both
61 the shift of the maximum pressure towards the geometrical focus at first, even passing
62 beyond the focus, and then the shift backwards to the transducer. They also provided an
63 interpretation of the phenomenon based on the self-defocusing effect due to the
64 asymmetrical distortion of the wave profile and to the increase in propagation velocity
65 of the compressive phase of the wave close to the beam axis.

66 The nonlinear focal shift phenomenon, as most of the characteristics of the high power
67 focused ultrasound beams, depends on the wave amplitude, the medium properties and
68 the source physical characteristics (frequency, aperture, and geometrical focal
69 length)^{14,15}. Two of them, the source physical characteristics and the wave velocity in
70 the medium, can be described through a single parameter, the Fresnel number. This
71 parameter, defined as $N_F = a^2 / \lambda F$, where a is the transducer radius, λ the wavelength and
72 F the geometrical focal length, is widely used in optics and allows classifying the sound
73 beams according to low ($N_F \sim 1$) or high ($N_F > 1$) focusing degree. As discussed in Ref.
74 13, the Fresnel number is proportional to the linear gain ($G = \pi N_F$), however, since due
75 to the linear focal shift phenomenon the real gain ($G_r = p_{max} / p_0$ where p_{max} is the on-axis
76 pressure maximum and p_0 the pressure in the surface of the transducer) is different from
77 G (linear gain), we adopt N_F to characterise the focusing of the sound beam in this
78 work. Note that G only estimates the magnification of the beam in the absence of focal
79 shift.

80 Table 1 shows the characteristics of the ultrasonic sources (and the corresponding
81 Fresnel number) used in previous studies related with the nonlinear focal shift
82 phenomenon. The table is arranged in increasing Fresnel number (last column), and
83 demonstrates the inverse relation between the Fresnel number and the magnitude of the
84 maximum pressure nonlinear focal shift normalised to the geometrical focal length
85 (Δ_{NL} ; penultimate column) as discussed in Ref. 13 from numerical solution of the
86 Khokhlov-Zabolotskaya-Kuznetsov (KZK) equation: the higher the focusing degree the
87 smaller the nonlinear focal shift.

88 Fig. 1 shows the maximum pressure nonlinear focal shift experimental results obtained
89 in the last decades (data from Table 1) and the KZK simulations (curve). The curve has
90 been performed by simulating different transducer geometries, from low amplitudes
91 (linear regime, ~ 20 kPa in the focus) to sufficiently large amplitudes ($\sim 4-5$ MPa in the
92 focus) to reach saturation in the maximum pressure shift, according to the procedure
93 followed in Ref. 13 (Fig. 6). A global agreement can be observed, even considering that
94 the experiments were not optimized for the observation of the nonlinear focal shift.

95 Although the nonlinear focal shift phenomenon has been observed and discussed in
96 previous studies⁸⁻¹⁴ for slightly focused beams, a specific study with the objective to
97 analyze, experimentally and numerically, the focal region of moderate Fresnel number
98 transducers ($4 < N_F < 8$) and the magnitude of this shift is absent, as can be seen in Fig. 1.

99 This is a focusing region of special interest because self-refraction plays a more
100 important role than in highly focused beams (like HIFU devices, where the volume of
101 the focus is too small to produce significant self-refraction effects) and in weakly
102 focused beams (where high voltages have to be applied to the transducer in order to
103 reach the amplitudes necessary to observe nonlinear effects). Also, numerical
104 simulations^{13,14} of moderate Fresnel number transducers predict that the on-axis
105 pressure maximum position could surpass the geometrical focal point due to the effect
106 of nonlinearity. We present the first experimental demonstration and explanation of this
107 phenomenon in the current study.

108 Additionally, a detailed analysis of the acoustic field of moderately focused beams, the
109 location of the significant points like maximum pressure, minimum pressure, maximum
110 intensity or maximum radiation force, as well as the nonlinear focal shifts may become
111 relevant in those applications where moderately focused ultrasound is used, as for
112 example in the transcranial ultrasonic propagation for the Blood Brain Barrier (BBB)
113 opening¹⁶, where typical focusing transducers are $N_F \sim 6$, or in thermal applications
114 which aims to widen the focal area to reduce the treatment times¹⁷ ($N_F \sim 10$).

115 Therefore, the aim of this work is to evaluate the nonlinear focal shift of an ultrasonic
116 beam with moderate Fresnel number ($N_F = 6$, with a corresponding linear gain $G=18.8$)
117 in pressure, intensity, and radiation force, as well as to demonstrate that the nonlinear
118 focal shift effect is able to move the real focus beyond the geometrical focus. The
119 pressure waveforms of the ultrasonic beam have been measured under linear and
120 nonlinear conditions and the spatial distributions of peak pressures, intensity, and
121 radiation force have been calculated. Numerical solutions based on the KZK equation
122 and known analytical solutions have been compared with experimental data. The
123 knowledge of the dynamic behaviour of the on-axis pressure, intensity, and radiation
124 force distributions provided in this work could be relevant to better characterize the
125 effects produced by ultrasonic focused beams in different medical applications as: HIFU
126 (maximum heat deposition), cavitation (negative pressure) or imaging¹⁸⁻²¹ (radiation
127 force).

128

129 **II. MATERIALS AND METHODS**

130 **A. Experimental Set-up**

131 The experimental setup follows the classical scheme of confronted emitting transducer
 132 and receiving calibrated membrane hydrophone in a 0.75×0.6×0.5-m water tank filled
 133 with degassed and distilled water, as shown in Fig. 2. The ultrasound source was
 134 formed by a plane single element piezoceramic crystal (PZ 26, Ferroperm
 135 Piezoceramics, Denmark) mounted in a custom designed steel housing and a
 136 methacrylate focusing lens with diameter 50 mm and radius of curvature $R=70$ mm. The
 137 resonant frequency of the system was 2.227 MHz, the radius $a=25$ mm and the
 138 geometrical focal length $F=157$ mm, obtained from the expression

$$139 \quad F = \frac{R}{1 - \frac{c_m}{c_l}}, \quad (1)$$

140 where c_m is the sound velocity in the medium (water), c_l the sound velocity in the
 141 methacrylate (2711 m/s) and R the lens radius of curvature²².

142 The transducer was driven with pulse bursts (150 cycles-sine wave bursts) using a
 143 function generator (14 bits, 100 MS/s, model PXI5412, National Instruments) and a
 144 linear RF amplifier (ENI 1040L, 400W, +55dB, ENI, Rochester, NY). To measure the
 145 acoustic waveforms a NTR PVDF membrane hydrophone (0.2229 V/MPa sensitivity,
 146 model MH2000B with 200 μm active diameter, NTR/Onda Corp.) and a digitizer (64
 147 MS/s, model PXI5620, National Instruments) were used. A three-axis micropositioning
 148 system (OWIS GmbH) was used to move the hydrophone in three orthogonal directions
 149 with an accuracy of 10 μm . All the signal generation and acquisition process was based
 150 on a National Instruments PXI-Technology controller NI8176, which also controls the
 151 micropositioning system.

152

153 B. Numerical model

154 Numerical modelling of the experiment was performed using the KZK equation for
 155 axi-symmetric beams^{23,24}:

$$156 \quad \frac{\partial^2 p}{\partial t^2 \partial z} = \frac{c_0}{2} \frac{\partial^2 p}{\partial r^2} + \frac{1}{r} \frac{\partial p^0}{\partial r} + \frac{d}{2c_0^3} \frac{\partial^3 p}{\partial t^3} + \frac{b}{2r_0 c_0^3} \frac{\partial^2 p^2}{\partial t^2} \quad (2)$$

157 where $t' = t - z/c_0$ is a retarded time, c_0 the sound propagation speed, δ the sound
 158 diffusivity, β the coefficient of nonlinearity, and ρ_0 the ambient density of the medium.

159 Equation 2 is valid in the paraxial approximation²⁵ ($F/a \gg 1$ and $ka \geq (F/a)^{\frac{1}{3}}$) and takes
 160 into account nonlinearity, diffraction and thermoviscous absorption. This equation is

161 solved by means of the numerical scheme described in Ref. 23. Equation 2 can be
 162 written in dimensionless variables as:

$$163 \quad \frac{\partial^2 P}{\partial \tau \partial \sigma} = \frac{1}{4G} \Delta_{\perp} P + A \frac{\partial^2 P}{\partial \tau^2} + NP \frac{\partial P}{\partial \tau} , \quad (3)$$

164 where $\tau = \omega_0 t'$ is the dimensionless time, $\sigma = z/F$ is the dimensionless axial
 165 coordinate, $\rho = r/a$ is the dimensionless radial coordinate, $P = p/p_0$ is the normalized
 166 pressure, Δ_{\perp} is the transversal laplacian operator, $G = z_d/F$ is the diffraction parameter
 167 or the gain, $A = F/z_a$ is the absorption parameter and $N = F/z_s$ is the parameter of
 168 nonlinearity. Here, $z_d = k a^2/2$ is the characteristic diffraction length (Rayleigh
 169 distance), $z_a = 2c_0^3/\delta\alpha_0^2$ is the characteristic absorption length and $z_s = c_0^3\rho_0/\beta p_0\omega_0$ is
 170 the plane wave shock formation distance.

171 Simulations were performed in water for beams of initially harmonic pulse burst waves
 172 with uniform pressure amplitude at the source. The acoustic source used in the present
 173 experiment meets the paraxial condition ($F/2a=3.1$), so the source condition for a
 174 moderately focused piston ($G=18.7$) can be modelled by means of delaying the time
 175 waveforms over the plane $z=0$, as²³:

$$176 \quad P(\sigma=0, \rho, \tau) = F(\rho, \tau + G\rho^2) , \quad (4)$$

177 where the source function $F(\rho, \tau)$ is defined as:

$$178 \quad F(\rho, \tau) = f(\tau)H(1-\rho) , \quad (5)$$

179 where $H(\rho)$ is the Heaviside step function defined in this case by $H(1-\rho)=1$ for
 180 $\rho \leq 1$ and $H(1-\rho)=0$ for $\rho > 1$, and $f(\tau)$ is the time delayed waveform (sinusoidal
 181 pulse burst). Thus, simulation parameters were $c_0=1486$ m/s, $\rho_0=998$ kg/m³, $\beta=3.5$,
 182 $\delta=5.13 \cdot 10^{-6}$ m²/s, $F=157$ mm, $a=25$ mm and 25 different values of p_0 ranging from 2
 183 kPa to 99 kPa. These physical parameters leads the dimensionless parameters of
 184 $G=18.7$, $A=0.024$, and 25 equally distributed values of N ranging from 0.0047 to
 185 0.2324. The algorithm described in Ref. 23 employs an operator splitting approach for
 186 solving the equation for an incremental step from σ to $\sigma + \Delta\sigma$. The numerical grid
 187 parameters were chosen small enough to ensure the solution does not vary less than 1%
 188 at halving the grid refinement. Thus, the time step chosen was $\Delta\tau=0.010$ and leads to
 189 200 samples per cycle, the transversal grid step was $\Delta\rho=10^{-3}$ and the axial grid step was

190 $\Delta\sigma_{IB}=10^{-4}$ for the fully implicit backward difference method, and $\Delta\sigma_{CN}=2\cdot 10^{-4}$ for the
191 Crank-Nicolson method. First method was applied to solve the field near the transducer
192 ($\sigma < 100 \Delta\sigma_{IB}$) and beyond this distance Crank-Nicolson method is applied.

193

194 **C. Measurement procedure**

195 In order to characterize the nonlinear focal shift phenomenon in the ultrasonic beam
196 emitted by the source it is necessary to measure the acoustic field on the radiator axis at
197 different initial pressures. Eight increasing and voltage inputs were applied at the
198 transducer terminals: $2 V_{pp}$ (linear regime), 9, 21, 45, 65, 85, 100, and $125 V_{pp}$, in order
199 to study the evolution of the acoustic field characteristics from linear to nonlinear
200 regime. The voltage values were selected to cover homogeneously the range. As the
201 beamwidth can be quite small (3 mm at the focus in the linear case, -6 dB), a precise
202 positioning of the hydrophone on the radiator axis is required. The axis of the radiator
203 was oriented approximately along the z -axis of the micropositioning system. Then, the
204 pressure waveforms $p(t,x,y,z)$ were measured in 25 planes along the z axis of the
205 micropositioning system: from 131.3 to 146.3 mm spaced each 3 mm; from 146.3 to
206 161.3 mm spaced each 1 mm; and from 161.3 to 176.3 mm spaced each 3 mm (see Fig.
207 3). These planes were transversal to the z axis, 6×6 mm (x - y planes) and waveforms
208 were acquired with 0.5 mm spatial resolution on them (144 measurement points/plane).
209 Five planes around the geometrical focus were acquired with 0.25 mm spatial
210 resolution. At every point of measure, waveform averaging was performed of multiple
211 tone burst to increase the signal-to-noise ratio. After that, the maximum of the
212 waveform signal was selected by adjusting a Gaussian function to the histogram of
213 maxima in the tone burst. The equipressure curves in each plane built with the selected
214 maxima typically had a circular form: this was indicative of good axial symmetry of the
215 radiator. Finally, from the measurement of the pressure maxima distribution in each x - y
216 plane we were able to obtain the pressure maximum amplitude and its coordinates
217 (x_{max}, y_{max}) in each of the 25 transversal planes, which allowed to define the radiator
218 axis.

219 As the hydrophone displacement along the axis was determined by the
220 micropositioning system with high accuracy (0.01 mm), to locate the hydrophone
221 position with respect to the radiator it was sufficient to measure the distance between
222 the receiver and the transmitter only at one point on the axis. This was done by

223 measuring the time passing between the tone burst front emission and reception, and
 224 using the value of the sound velocity at the temperature of water. The accuracy of this
 225 measurement was better than 0.3 mm.

226 Most of the measured planes were located close to the geometrical focus location with
 227 minimal separation of 1 mm between them (see Fig. 3). This spatial resolution in z was
 228 especially necessary in order to evaluate the position of the on-axis pressure maximum
 229 with an accuracy better than 3 mm, which is the requirement to be sensible to the
 230 nonlinear pressure focal shift phenomenon (estimated in less than 1 cm from numeric
 231 simulations, Makov et al.¹³). In spite of the fact that we measured the on-axis pressure
 232 maximum every 1 mm near the geometrical focus, as the measurement of pressure had a
 233 random error estimated from 2% (lower pressure) to 4% (higher pressure) in our
 234 experiment, the uncertainty in the determination of the location is higher than 1 mm, as
 235 shown by the error bars in the different plots (Fig. 5, 8 and 9).

236 To evaluate the on-axis intensity $I(z)$ and radiation force $F(z)$ distributions the
 237 temporal profiles $p(t, z)$ have been used in the following expressions.

238 For the intensity:

$$239 \quad I(z) = \frac{1}{nT} \int_{t_0}^{t_0+nT} \frac{p^2(t, z)}{\rho c} dt, \quad (6)$$

240 where T is the period, n is an integer, ρ is the water density and c is the speed of sound.

241 And for radiation force²⁶:

$$242 \quad F(z) = \frac{b}{c^5 \rho^3} \left\langle \left(\frac{\partial p(t, z)}{\partial t} \right)^2 \right\rangle, \quad (7)$$

243 where b is the dissipation and the angular brackets denote temporal averaging over fast
 244 acoustic oscillations.

245

246 **D. Linear characterization of the beam**

247 The characterization of the beam in linear regime is needed to determine the
 248 characteristics of the acoustic source (aperture and geometrical focus) and the position
 249 of the on-axis pressure maximum, i.e., the linear focal shift. The linear characterization
 250 was performed in three steps: first, nominal values (those provided by the lens
 251 manufacturer) were used to evaluate the nominal geometrical focal length according to
 252 Eq. 1. Next, the analytic O'Neil solution¹, valid for linear focused fields, was fitted to
 253 the experimental data at the lower voltage excitation value of the transducer ($2 V_{pp}$).

254 This fit provided a new value for the geometrical focal length and aperture, and a value
255 for the pressure in the source, $p_0 = 2$ kPa. Finally, KZK simulations were performed for
256 various values of the source aperture and radius of curvature to obtain the “best fit” to
257 the experimental data in the linear regime.

258 The geometrical focal length and the aperture of the transducer were nominally stated
259 by the manufacturer as $F = 157$ mm and $2a = 50$ mm, respectively, resulting in $N_F = 6$
260 (being 2.227 MHz the working frequency), f-number = 3.14, and $G = 18.8$. The fit of
261 the analytic O’Neil solution to the experimental data is shown in Fig. 4.a, and provides
262 an effective aperture of the transducer of 51.6 mm and an effective geometrical focal
263 length of 158.2 mm. Fig. 4.b shows a good behavior of the fit also in the transversal
264 distribution of the pressure. And finally, the KZK simulation provides an effective
265 aperture of the transducer of 50.2 mm, and a geometrical focal length of 157 mm. The
266 small differences between all three calculations can be due to the fact that linear KZK
267 and O’Neil solutions are different as they are solutions of different diffraction models
268 (parabolic approximation and Rayleigh integral) and to the fact that our transducer is
269 not a perfect piston: the transducer housing, the surface waves and the effect of the lens
270 borders might limit and distort its vibration⁸.

271 The on-axis pressure maximum obtained in the experiment is located at 154 mm from
272 the transducer, i.e. 97.8 % of the geometrical focal length, what is in good agreement
273 with the value of the linear focal shift predicted in Ref. 13 for transducers with Fresnel
274 number 6, i.e. 97%. The results of both models, the O’Neil and the calculated with the
275 “best fit” aperture and geometrical focal length in the KZK simulation, are in good
276 agreement with the experimental data.

277 Finally, the values of aperture and geometrical focal length obtained by the “best fit”
278 between the experimental values and the KZK simulated values in linear regime will be
279 used to simulate the acoustic field in the nonlinear regime.

280

281 **III. RESULTS**

282 To study the effect of the nonlinear propagation on the on-axis distribution of the
283 pressure, intensity, and radiation force, acoustic waveforms in front of the emitter were
284 acquired (as described in section II.C.) for different input voltage applied to the
285 transducer (from 2 V_{pp} to 125 V_{pp}). Fig. 5 shows the value and location of the on-axis
286 maximum and minimum pressure measured experimentally (dots). Error bars in the

287 estimation of the maxima locations are due to the errors associated to the measurement
288 of the pressure in our experiment. They range from 1 mm in the linear case ($2 V_{pp}$) to 3
289 mm in the higher excitation case ($125 V_{pp}$), increasing with the voltage input because
290 the transversal area (beam waist) of the focus becomes thinner (see Fig. 9) and it is
291 increasingly difficult to estimate the value of the maximum pressure in each transversal
292 plane (0.25 mm transversal spatial resolution and 0.2 mm hydrophone active diameter),
293 what implies an increasing of the error in the determination of the axial position of the
294 different maxima. Error bars in the determination of the minima locations are invariant:
295 1 mm, the minimum distance between the measured planes, as the beamwidth of the
296 negative focus increases with the excitation voltage (see Fig. 9).

297 The vertical line in Fig. 5 represents the position of the geometrical focus ($F = 157.4$
298 mm), estimated as the mean of the three values obtained in section A with independent
299 methods. The curves represent the on-axis maximum (continuous) and minimum
300 (dashed) pressure values and locations evaluated from the KZK numerical simulation of
301 the experiment. Both, experiment and simulation show the same four relevant
302 conclusions: 1) the on-axis pressure maximum position moves away from the
303 transducer when the exciting power increases (until 7.5 mm, corresponding to 4.8% of
304 nonlinear focal shift; see Fig. 1), 2) the on-axis pressure minimum position moves
305 towards the transducer when the exciting power increases (6.2 mm), 3) the on-axis
306 pressure maximum can surpass the position of the geometrical focus and 4) at the
307 highest excitation voltage ($125 V_{pp}$), the distance between the maximum and the
308 minimum pressure is larger than 1 cm.

309 The behavior of the maximum and minimum pressure positions presented in Fig. 5 can
310 be understood considering the effect of self-refraction²⁷ associated to nonlinear
311 propagation. Since the velocity of finite amplitude waves grows with the value of the
312 amplitude, and in a focused beam the amplitude is higher along the propagation axis
313 than in remote regions, the compressive phase of the waves travel faster near the axis.
314 Consequently, a flattening of the wave front is produced, leading to a displacement of
315 the pressure maximum from the source. The contrary effect is produced for the
316 rarefaction phase of the waveform (self-focusing). Due to the asymmetric distortion of
317 the wave profile caused by the combined effects of nonlinearity and diffraction, the
318 propagation velocity of the rarefaction phase decreases on the axis (and the focus)²⁴

319 causing an additional focusing of the waveform, and consequently a displacement of the
320 maximum rarefaction pressure towards the source.

321 Fig 6 shows a simple (ray theory and Snell law) representation of the self-refraction
322 effect for the positive and negative peak pressures. For illustrative purposes, it has been
323 considered that the change in the wave speed is due to a change in the propagation
324 medium (different medium in the paraxial area near the focus), although the effect is
325 due to nonlinear effects. The rays are defocused (b) or focused (c) with respect to the
326 linear case (a) due to the change in the propagation velocity. If the transducer is strongly
327 focused, the focal region becomes too small to produce significant self-refraction
328 effects, which is the reason why HIFU instruments do not suffer large nonlinear focal
329 shift effects.

330 Experimental and simulated values in Fig. 5 show good agreement in the quasi-linear
331 region (lower input voltages) but they differ slightly as the power increases (nonlinear
332 regime), being the nonlinear focal shift effect higher in the simulation. There are several
333 possible reasons that explain this fact: first, the frequency response of the hydrophone is
334 bounded to 20 MHz, which limits the number of affects harmonics detected by the
335 hydrophone. Second, the sound field does not present a flat and uniform distribution
336 over the active area of the receptor (200 μm active diameter), thus the measure is
337 underestimated after the spatial averaging of the measurement region, on the contrary,
338 the simulation maximum are the KZK solution for an infinitesimal field point. A final
339 source of error is due to the non-uniform vibration of the transmitter, as discussed
340 before. These hypotheses have been discussed in detail in Ref. 8. In our case, the finite
341 size of the hydrophone was simulated by averaging over a 200 μm diameter circular
342 cross section, equivalent to active hydrophone diameter. The results show that spatial
343 averaging of the hydrophone sub-predicts the positive peak pressure. The magnitude of
344 the discrepancy linearly varies from 0.6% for low input pressures to 2.1 % for 3.7 MPa
345 peak pressures. The finite bandwidth of the hydrophone was simulated by zero-phase
346 filtering the KZK signals by a low pass filter equivalent to the frequency response of the
347 hydrophone. The nonlinear focal shift processed by the filtered signals is sub-predicted
348 and matches the experimental results. These results evidence that the limited bandwidth
349 of the receiver alter the measurement of the beam properties, i.e. the effect of focal
350 displacement will be stronger if all harmonics are recorded. Thus, filtering the simulated
351 waveforms with a 20 MHz low pass filter the estimations on the focal displacements

352 varies -1.3% for 3.6 MPa and the peak pressure value varies -6% for 3.6 MPa. Using
353 these uncertainties, the simulated-limited finite size and bandwidth of the hydrophone
354 predictions agrees the experimental measurements and its order of magnitude is
355 comparable to that measured in other papers⁸.

356 Fig. 5 shows saturation in the on-axis pressure maximum shift. At these intensities, a
357 high amplitude shock develops near the focus (see Fig. 7(d)). Nonlinear absorption of
358 the wave energy occurs at the shocks and the peak positive pressure decreases,
359 diminishing the self-refraction effect. The saturation effect is not observed in the on-
360 axis rarefaction maximum because the nonlinear absorption affects mainly the higher
361 frequencies (the narrow positive peak).

362 Previous studies demonstrate that the on-axis pressure maximum shifts towards the
363 source at very high intensities, after saturation is reached (numerically^{9,14,28} and
364 experimentally⁹). This is due to the presence of shock waves in the prefocal area, where
365 the nonlinear absorption decreases the wave amplitude and consequently reduces the
366 self-defocusing effect.

367 Fig. 8 shows the value and location on the on-axis maximum intensity and radiation
368 force. Intensity, evaluated from Eq. 6, reach a maximum at 120 W/cm^2 , which is far
369 away from the typical values that can be obtained with HIFU devices. A small shift in
370 the location of the on-axis intensity maximum is observed in the KZK simulation (2.3
371 mm) that agrees with the experimental results, although the error in the estimation of the
372 intensity location is higher than the shift. Previous studies show the same singular
373 behaviour for the intensity¹³: the shift is always smaller than in pressure and it decreases
374 with the focusing degree of the source. At very high focusing levels (HIFU devices, for
375 example) the shift is insignificant and the on-axis intensity maximum is located at the
376 geometrical focus. However, the radiation force is very sensible to the self-refraction
377 effect. As it can be seen in Fig. 8, the shift is comparable to that observed for the
378 pressure (Fig. 5), both in the experiment and the simulation, even surpassing the
379 geometrical focus. This effect can be important in ultrasound-stimulated vibro-
380 acoustography techniques¹⁸⁻²¹ (where the radiation force is used to produce
381 displacements in tissue), as the location where the radiation force is applied can change
382 with the amplitude of the excitation wave.

383 It is important to indicate that the on-axis pressure maximum, pressure minimum,
384 intensity, and radiation force show different behaviour under increasing nonlinearity.

385 On-axis maximum and minimum pressure shift behaviour has been explained by the
 386 self-refraction effect, which can also explain the saturation in the maximum pressure
 387 shift due to the nonlinear absorption that appears in the shock waves. As mentioned, the
 388 shift in radiation force is very similar to the shift in maximum pressure: radiation force
 389 is proportional to the absorption, which increases with frequency, therefore both will be
 390 higher in distorted wave profiles (with more harmonics), which correspond to the more
 391 peaked waveforms (higher positive pressure).

392 However, a different behaviour can be observed in the intensity shift, much smaller
 393 compared with the maximum pressure shift. The character of the nonlinear deformation
 394 of time profiles shown in Fig. 7 provides the clue to understand this discrepancy during
 395 the process of nonlinearity development. Actually, the deformation of the time profile
 396 lies in the quite fast increase of the profile peak level together with the simultaneous
 397 narrowing of this peak, as observed in Fig. 7. This dynamic process is accompanied by
 398 a deceleration in the increase of the area under this peak. Under the condition⁶

$$399 \int_0^T p(t,x,y,z)dt = 0, \quad (5)$$

400 the comparative growth of the area of the negative part of the profile is also decelerated,
 401 and the intensity (as the square of the full area under the curve profile, see Eq.(3))
 402 slows down¹³. This becomes apparent in the lag of nonlinear shift of the intensity
 403 maximum compared with the shift of pressure maximum.

404 As nonlinear effects increase, not only the locations of spatial maxima of pressure,
 405 intensity, and radiation force change, but also the transversal spatial structure²⁴. Fig. 9
 406 shows the compression and the rarefaction beamwidth in the geometrical focus at a
 407 level of -6 dB in the transverse direction for the different input voltages. In the focal
 408 area, compression beamwidth decreases in nonlinear regime (-36 %) meanwhile
 409 rarefaction beamwidth increases (+36 %). This is due to the way nonlinearity distorts
 410 the wave in the presence of diffraction. The wave acquires a frequency-dependent phase
 411 shift. This leads to the appearance of corresponding phase shifts between the harmonics,
 412 which produces an asymmetric profile distortion: within each period, the compression
 413 region becomes higher and sharper and the rarefaction region becomes smoother (see
 414 Fig. 7(c and d)). The asymmetric profile distortion of the waveform is the responsible of
 415 the increase of the real gain (p_+/p_0) in the moderate nonlinear region and the decrease of
 416 the negative real gain ($p-/p_0$) respect to the linear gain value⁸. So, the maximum pressure
 417 grows faster in the region near the focus (where the higher distorted waveforms are

418 located) than in the off-axis regions when input excitation in the transducer increases,
419 reducing the positive beamwidth (and consequently the transversal area of the focus).
420 Contrary, the rarefaction regions of the wave grows more slowly in the propagation axis
421 (and in the focus) than in the regions around the focus because the waveform is more
422 distorted on axis, so the transversal amplitude profile becomes flattened when
423 nonlinearity is higher, increasing the rarefaction beamwidth.

424

425 **IV. CONCLUSION**

426 The acoustic field of a moderately focused transducer ($N_F = 6$; $G = 18.8$; f-number =
427 3.14) has been studied in order to determine the characteristics of the linear and
428 nonlinear focal shift in the case of pressure, intensity and radiation force.

429 In linear regime it has been observed that the on-axis pressure maximum is located at
430 154 mm from the transducer, i.e. before the geometrical focus (157.4 mm), which
431 indicates a linear focal shift of 3.4 mm. This shift agrees with the Makov et al.¹³ results
432 in their study about the dependence of the linear focal shift with the Fresnel number.

433 In nonlinear propagation conditions it has been observed a maximum pressure position
434 displacement (both in experiment and simulation) when the input voltage is increased,
435 even exceeding the geometrical focus. It has also been observed a shift in the on-axis
436 pressure minimum, but in the contrary direction (backward). This behaviour has been
437 explained by means of the effect of self-refraction, that modify the focusing conditions
438 respect to the linear case. When the maximum voltage is applied to the transducer the
439 on-axis pressure maximum position exceed the geometrical focus in 4 mm, and the
440 separation between the on-axis maximum and minimum positions is as far as 13.7 mm.

441 The on-axis intensity maximum is located in the linear regime at the same point than
442 the on-axis maximum and minimum pressures (154 mm from the transducer). There is a
443 shift in the position of the maximum intensity when the input voltage to the transducer
444 increases, but it is quite low (2.3 mm) compared to the shift in the pressure (7.5 mm),
445 and it does not surpass the geometrical focus. The reason for the different behaviour
446 between them has been explained on the base that the fast growth of the positive peak in
447 a period does no imply an increase in the area subtended by this period (and
448 consequently the intensity).

449 However, the radiation force follows the same behaviour than the maximum pressure
450 because the sharper the positive peak the higher the absorption, increasing the value of
451 the force applied to the medium.

452 There exists a spatial separation between the points of interest in a beam: maximum
453 pressure, minimum pressure, intensity, and radiation force, that depends on the Fresnel
454 number and input voltage applied to the transducer. From the results of this work, at the
455 higher input voltage applied, the maximum pressure and the maximum radiation force
456 are located at 161.5 mm from the transducer, the minimum pressure is located at 148
457 mm and the maximum intensity at 156.3 mm. This dissociation between the relevant
458 points in an ultrasonic beam implies that the effects produced will be also spatially
459 dissociated, what has to be taken into account according to the desired application. In
460 thermal applications of ultrasound²⁹ the pressure waveform is important as it determines
461 both, the radiation force and the heat deposition in the medium; rarefaction is
462 responsible of cavitation, so the minimum pressure location will be the region of
463 interest in applications where cavitation takes an important role, as for example in
464 transcranial Blood Brain Barrier (BBB) opening¹⁶. Finally, radiation force is used in
465 new elastographic techniques as HMI²¹ or ARFI²⁰ to induce displacements of the tissue
466 in the focus of the beam, so that the knowledge of the exact position of the on-axis
467 maximum radiation force applied is crucial.

468 The nonlinear focal shift studied in this work becomes less important in highly
469 focused beams (as for example, in HIFU devices) because the focal area is smaller and
470 self-refraction effect decreases. However, detailed studies should be conducted if the
471 technique is very sensible to the value and location of the radiation force applied, as it is
472 the case of acoustic radiation force elastography techniques³⁰.

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474

475 **ACKNOWLEDGMENTS**

476 We wish to thank Dr. Yuri N. Makov for his advices and remarks for the improvement
477 of this article. This work was supported by Universitat Politècnica de València, under
478 the projects PAID-06-10-002-295 and PAID-05-11-002-340.

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558 Table I. Historical studies where nonlinear focal shift evidences have been reported.

559 Water has been used in all the experiments.

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561

<i>Reference</i>	<i>Source Characteristics</i>			<i>Nonlinear focal shift p_+</i>	<i>Nonlinear focal shift p_+</i>	N_F
	<i>Freq. (MHz)</i>	<i>Radius (mm)</i>	<i>Focus (mm)</i>	<i>(mm)</i>	<i>(Δ_{NL}) (%)</i>	
Makov <i>et al.</i> ⁹ , 2006	1	15	117	24	20	1.28
Duck <i>et al.</i> ¹¹ , 1986	3.5	6.5	70	15	21	1.4
Duck <i>et al.</i> ¹¹ , 1986	2.25	9.8	90	~17	19	1.51
Duck <i>et al.</i> ¹¹ , 1986	5	6.5	80	~8	10	1.8
Averbukh <i>et al.</i> ¹²	2.25	18.8	160	~11	7	3.34

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575 FIGURE CAPTIONS

576 Fig. 1. Nonlinear focal shift in the maximum pressure evaluated in different
577 experiments from 1986 to actual date. The dot represents the result obtained in the
578 present study.

579

580 Fig. 2. Scheme of the experimental set up for the pressure measurement in water.

581

582 Fig. 3. Measuring procedure. Waveforms are measured in 25 planes along the z axis of
583 the micropositioning system. The slice separation was $d_1=3$ mm and $d_2=1$ mm.

584

585 Fig. 4. a) On axis pressure distribution and b) transversal normalized pressure in linear
586 regime.

587

588 Fig. 5. On axis maximum positive and negative pressures. Experimental values and
589 KZK simulation. Input voltage values are 2, 9, 21, 45, 65, 85, 100 and 125 V_{pp} from
590 bottom to top.

591

592 Fig. 6. Geometrical interpretation of the self-refraction phenomenon. Ray theory is
593 considered in the graphs. In a) the absence of diffraction makes the transducer focus in
594 the geometrical focus in linear regime. In b) the positive peak are defocused because of
595 the increase of velocity in this phase of the waveform in nonlinear regime, and in c) the
596 rarefaction phase of the waveform is focused prefocally because the decrease of the
597 velocity.

598

599 Fig. 7. Time profiles in the geometrical focus at different input voltage.

600

601 Fig. 8. On-axis maximum intensity and radiation force. Experimental values (dots) and
602 KZK simulation (curves).

603

604 Fig. 9. Compression and rarefaction beamwidth (defined at -6 dB) at the geometrical
605 focus for the different input voltages applied: 2, 9, 21, 45, 65, 85, 100 and 125 V_{pp} from
606 bottom to top. Experimental values (dots) and KZK simulation (lines).

607