1.1 Theoretical considerations

The history of nonlinear acoustics can be traced back nearly 250 years to Euler's equations for momentum and continuity of motion in a fluid [[i]]. Since this beginning a great deal of literature has been published by some of the most distinguished scientists in the 18th, 19th & 20th centuries. A detailed historical review of the beginnings of nonlinear acoustics (1755 - 1930) can be found in Hamilton and Blackstock's Nonlinear Acoustics [[ii]]. Following on from this period, several key theories describing the various effects of nonlinear waves under certain conditions emerged. The three most widely accepted and respected equations describing nonlinear propagation were formulated by Burgers, Westervelt and the trio Khokhlov, Zabolotskaya and Kuznetsov (KZK). Each of these individual descriptions of nonlinear propagation all feature a parameter known as the nonlinearity parameter, ß.

1.1.1.1 The Nonlinearity Parameter

The nonlinearity parameter, ß, determines the nonlinear effect on wave propagation. It is defined in Equation 5.1, where the ratio B/A describes nonlinearities in the medium.

$$\beta = \begin{cases} 1 + B/2A & \text{for liquid} \\ (\gamma + 1)/2 & \text{for gas} \end{cases} \qquad 5.1$$

where γ = ratio of specific heat co-efficient at constant pressure and volume (c_p/c_v)

The quantity *B/A* is the pivotal aspect of the relation as it has a significant effect on sound speed. It can be expressed in terms of thermodynamic quantities [ii] as Equation 5.2.

$$\frac{B}{A} = 2\rho_o c_o \left(\frac{\partial c}{\partial p}\right)_T + \frac{2\alpha_T c_o T_o}{c_P}\left(\frac{\partial c}{\partial T}\right)_p \qquad 5.2$$

where c_o = small signal velocity of sound

c = local velocity of sound in the wave

ρ_o = fluid density

T_o = absolute fluid temperature

α_T = coefficient of thermal expansion

c_P = specific heat capacity at constant pressure

In effect, the quantity B/A will vary depending on the temperature, pressure and density of the medium through which a finite amplitude sound wave is propagating. Examples of this quantity for two common load media are as follows; distilled water has a ratio B/A = 5 and air has B/A = 0.4, both calculated at a temperature of 20°C

1.1.1.2 Westervelt Equation

The Westervelt equation is an approximation of the second order wave equation and describes the propagation of a nonlinear, quasi-planar sound wave. The derivation of the equation is from that of a thermoviscous fluid perspective incorporating expansions of mass conservation, momentum conservation, entropy balance and thermodynamic state equations. There are certain assumptions embedded within the derivation of the equation, primarily that the propagation medium is homogenous in composition and its unperturbed density and pressure are uniform. There are others involved but these are more in context within fluid dynamics and are therefore not mentioned in this work. Equation 5.3 represents the Westervelt equation [ii].

$$\left(\nabla^2 - \frac{1}{c_o}\frac{\partial^2}{\partial t^2}\right)p + \frac{\delta}{c_o^4}\frac{\partial^3 p}{\partial t^3} + \frac{\beta}{\rho_o c_o^4}\frac{\partial^2 p^2}{\partial t^2} = 0 \qquad 5.3$$

where ∇^2 = Laplacian operator

δ = diffusivity of sound (absorption in the medium)

p = change in ambient pressure

The expression can be broken down into three unique terms. The first two terms (in parenthesis) represent diffraction and linear propagation and are the wave equation for linear propagation. The third term describes thermoviscous losses in the fluid, or in other words, absorption in the medium. Finally, the last term accounts for the nonlinear effect on wave propagation and is governed by the nonlinearity parameter, β.

1.1.1.3 Burgers Equation

The Burgers equation is one of the fundamental equations in nonlinear acoustics. It is the simplest model that describes the combined effects of nonlinearity and loss on the propagation of progressive plane waves. It can be derived from the 1D form of the Westervelt equation and is represented in Equation 5.4 [ii].

$$\frac{\partial p}{\partial z} = \frac{\delta}{2c_o^3}\frac{\partial^2 p}{\partial t^2} + \frac{\beta p}{\rho_o c_o^3}\frac{\partial p}{\partial t} \qquad 5.4$$

The equation can be split into two parts; the first term on the RHS describes dissipative effects and the second term nonlinear effects. For small amplitude waves the nonlinear parameter can be ignored, $\beta=0$, therefore leaving only dissipative effects left to describe wave evolution. Given this, for a homogenous medium, the propagation of a harmonic wave is described by a solution with exponentially decreasing amplitude [iii]. For the case when dissipative effects are negligible, δ=0, only a solution for the nonlinear aspect is available. These particular solutions are shown in Equations 5.5 and 5.6 respectively [ii].

$$p = p_o \exp\left[\mathbf{j}\omega\tau - \left(\delta\omega^2 / 2c_o^3 \right) z \right] \qquad 5.5$$

$$p = f\left[\tau + \left(\beta p / \rho_o c_o^3 \right) z \right] \qquad 5.6$$

Equation 5.6 is sometimes referred to as the Earnshaw/Poisson solution to Burgers equation. An in-depth historical review of the Burgers equation is available in Hamilton and Blackstock's Nonlinear Acoustics [ii]. A more general form of the Burgers equation, in spatial representation, can be found in Naugolnykh and Ostrovsky's nonlinear wave processes in acoustics [iii].

1.1.1.4 KZK Equation

The KZK equation is an augmentation of the Burgers equation that accounts for the combined effects of diffraction, absorption and nonlinearity in directional sound beams. Equation 5.7 represents the nonlinear parabolic KZK equation [ii].

$$\frac{\partial^2 p}{\partial z \partial t} = \frac{c_o}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) p + \frac{\delta}{2c_o^3}\frac{\partial^3 p}{\partial t^3} + \frac{\beta}{2\rho_o c_o^3}\frac{\partial^2 p^2}{\partial t^2} \qquad 5.7$$

The first term on the RHS describes the effects of diffraction where the expression in parenthesis is the transverse Laplacian operator, $\nabla_\perp^2$, which is equivalent to Equation 5.8. The second term describes the effects of dissipation on a travelling wave.

Finally, the third term describes nonlinear effects on the evolution of a propagating sound wave.

$$\nabla_{\perp}^{2} = \nabla^{2} - \frac{\partial^{2}}{\partial z^{2}} \qquad 5.8$$

The KZK model assumes that the acoustic energy propagates in a fairly narrow beam close to the source axis up to around 20° off the z-axis in the far field. Moreover, the approximation is valid for field points that are beyond a few source radii and regions that are not too close to the source plane. The assumption to be satisfied for a circular, piston-like source of radius *a* and wavenumber *k*, is that $ka >> 1$. Hence ensuring that the beam is reasonably directional, angular spectrum is narrow and therefore wavefronts are quasi-planar [**Error! Bookmark not defined.**, i & [iv]]. The KZK equation is the most widely used model for describing all three effects on the development of a travelling acoustic wave in a homogenous medium, with solutions in the time domain and spectral domain having been developed [[v], [vi]].

1.1.2 Analytical Approach

Due to the KZK model's ability in describing the evolution of a travelling wave distorted by the effects of diffraction, absorption and nonlinearity within certain limitations, a number of computer algorithms have been proposed to solve the KZK equation numerically. The first approach developed was a frequency domain method, often called the spectral technique, formulated by Aanonsen and co-workers [vi]. The KZK can be solved in the frequency domain for monochromatic or tone burst signals by using a finite difference scheme to propagate the wave forward in small steps. Essentially, the pressure wave can be written in terms of Fourier components consisting of the fundamental and its harmonics, truncated at the Nth harmonic to reduce calculation burden, and then substituted into the KZK equation. This enables a set of coupled equations to be derived that allow each harmonic at a grid point in the (x,y) plane at a distance $z + \Delta z$ to be written in terms of the harmonic amplitudes at z. The computational procedure for solving these equations can become very time intensive for a distorted waveform involving N harmonics as the calculation of each harmonic, at each grid point, will involve N^2 multiplications. This problem is further compounded if frequency dependent absorption and strongly focused beams are to be accounted for in the prediction. Furthermore, if source excitation comprises of transients signals, or pulses, then a sufficiently low pulse repetition rate is required to ensure that adjacent pulses in the sequence do not overlap as a result of potential lengthening in duration due to absorption and nonlinearity, otherwise computational burden can be increased by an order of 100.

The spectral approach was followed by a more generic technique in the time domain proposed by Hamilton and Lee [v]. The solving of each term in the KZK model in the temporal domain significantly eases the strain imposed on computational resources by frequency domain solutions, primarily as the nonlinear term can now be solved with a computational time proportional to N as opposed to N^2. In addition, the need to implement Fourier transforms is removed. A marching scheme based on evaluating each of the effects individually was used as the basis for this solution.

1.1.3 Finite Element Approach

Despite the excellent agreement achieved between results from experiment and models based on the KZK equation [iv-vi], these algorithms remain too idealised for application to more complicated problems involving scattering, cavitation and medium inhomogeneities. A more useful approach modelling non-linear propagation in a load is to implement an incrementally linear solution to the governing elasticity equations [i]. In effect, for transient phenomena this process involves advancing a solution in time by small, discrete steps and modifying material properties according to the new state of the material. These time increments are minute enough that the solution is linear over each step and ensures wave nonlinearities are well-modelled by the incrementally linear approach. This technique, i.e. the constant repetition of simple calculations, is ideally suited to numerical solution using FEM code, specifically, the PZFlex package. The code implements a model based on [**Error! Bookmark not defined.**]

$$p = p_o + \rho_o c_o^2 \left[\left(\frac{\rho - \rho_o}{\rho_o} \right) + \frac{B}{2A} \left(\frac{\rho - \rho_o}{\rho_o} \right)^2 \right] \qquad 5.9$$

This allows a selected region of the grid, which is non-piezoelectric in nature, to be allocated material properties that support nonlinear propagation under the correct conditions, i.e. sufficient pressure amplitudes and/or distance from source. Importantly, this allows nonlinear behaviour to be simulated by FE analysis using PZFlex.

The large majority of literature on nonlinear propagation and simulation techniques focuses on the use of ultrasound in medical applications that operate at relatively high frequencies (2-10MHz). At these frequencies, sufficient pressures for harmonic creation are easy to generate at small input levels, where pressure is proportional to particle displacement (or velocity) and frequency, as such

$$P = \rho_o c_o \omega \xi \qquad 5.10$$

where: ξ = particle displacement

In addition, the associated reduction in wavelength allows for large propagation distances, in terms of number of wavelengths, over a small range. Therefore, in water and biological samples, it is fairly easy for the evolution of a pressure wave to deviate from its pure sinusoidal form. However, at the much lower frequencies that favour the generation of cavitation (20–100kHz), it is not so easy to generate the pressure levels, or transmission distance, in the load required for the initiation of nonlinear behaviour, with the obvious exception of SONAR. This creates an interesting scenario when investigating the pressure fields generated in the test vessels used prevalently in industrial processing applications, in that it may be possible to stimulate cavitation while the system effectively remains in the linear regime. Indeed, it is not unreasonable to postulate that the generation of harmonics in this situation may be more of a hindrance when attempting to maximise cavitational events due to the fundamental frequency 'leaking' energy to the higher frequencies.

It is often assumed that due to the high input levels associated with ultrasound in many process and ultrasonic cleaning applications, nonlinear waveforms will be readily generated. The presence of harmonics due to nonlinear propagation can have a profound impact on the field profile, causing it to deviate from the linear profile. Therefore, for the accurate characterisation of such acoustic fields it is important that nonlinear effects, if any, can be well-represented. Simulation of these effects in the ultrasonic system described in Section 4.4 is possible through inclusion of a transmission load that supports nonlinear effects in the model. As PZFlex cannot represent piezoelectric nonlinearities caused by high input voltages, any harmonics produced in the load medium would arise due to acoustic activity simulated within the vessel. However, in practice, equipment and device nonlinearities may exist and contribute to the acoustic field. It should be noted that these effects are separate from the nonlinearities associated with the onset of cavitation, both inertial and non-inertial, where bubble oscillations can generate harmonics and sub-harmonics of the fundamental frequency, and where bubble implosions can produce broadband acoustic pulses. These are also not represented directly by PZFlex, although potential simulation methods to emulate cavitation and its affect on the field profile will be discussed later in Chapter 7.

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