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Formation of Rarefaction Shockwaves in Non-ideal Gases with Temperature Gradients

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Abstract. The nonlinear propagation of finite amplitude waves in the non-ideal compressible fluid dynamic (NICFD) region of high-molecular weight fluids, and in particular in cases where non-classical gas dynamic phenomena like the formation of rarefaction shock waves may be expected, is of great scientific interest. Almost all the theoretical developments so far are based on the assumption that the waves propagate in a fluid kept in homogeneous conditions. Experimental activities performed with the Flexible Asymmetric Shock Tube (FAST) operated in the laboratories of the Propulsion and Power group at the Delft University of Technology have shown that obtaining such conditions is particularly challenging, especially keeping the tube at constant temperature. Stemming from this observation, this study is a part of a theoretical and numerical investigations aimed at assessing the influence of temperature gradients at the boundary on wave propagation in so-called Bethe-Zel'dovich Thompson (BZT) fluids. The full-wave Westervelt Equation is solved numerically using the Finite Difference Time Domain (FDTD) method. The steepening of the wave front is used as an indicator of shock formation. The effect of varying temperature, and the corresponding variation of the fundamental derivative of gas dynamics on the distortion of rarefaction waves is analyzed by observing the simulated behaviour of the wave as it propagates from a region of negative values of the fundamental derivative of gas dynamics to a region of positive values.

Keywords: NICFD · BZT · Γ · Non classical gas dynamics · Rarefaction shockwaves · Westervelt equation · Nonlinear distortion

1 Introduction

Non-ideal compressible fluid dynamics (NICFD), and non-classical fluid dynamics within it, have been rather extensively studied theoretically, numerically and experimentally. Most of the studies on non-linear wave propagation in the NICFD regime are based on the assumption that the medium in which the waves travel is in homogeneous conditions. All the so-far unsuccessful experimental efforts aimed at generating and measuring the formation and propagation of rarefaction shock waves in the dense vapor of BZT fluids [1,4,9] also relied and rely on trying to obtain such conditions in order to facilitate the interpretation of experimental results. However, obtaining a sufficiently constant temperature at the surfaces of the volume containing the fluid is challenging. For this reason, but also and more in general, to expand the theory of non-linear

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wave propagation in the NICFD regime, it is of interest to extend the modeling of wave propagation in non-homogeneous fluids to the case of dense vapors of fluids exhibiting negative values of the fundamental derivative of gas dynamics Γ for the thermodynamic states of the fluid affected by the process.

Γ is very sensitive to variations in temperature, therefore a small change in the temperature of the medium can give rise to a completely different nonlinear behaviour of the propagation of the waves. Such propagation is affected by strong effects on the steepening of a nonlinear distortion as the wave progresses through regions of opposite nonlinearities.

An important parameter for the experimental study of nonlinear wave propagation is the shock formation distance. For a uniform medium, this can be computed easily using the method of characteristics (MoC) [2,9]. In this case, the characteristic lines are straight with constant slopes and their intersection indicates shock formation. The MoC is both more complex to solve and exhibits some limitations when the temperature of the fluid varies, in which case the characteristic lines are curved due to the changing value of the local sound speed. In such situations, a more general approach to describe the nonlinear evolution of a disturbance needs to be employed.

The nonlinear steepening of waves in a medium with an axial variation in temperature, and thus a variation in Γ, is investigated using the full-wave Westervelt Equation. The Westervelt equation is a well-known mathematical model in nonlinear acoustics, widely used in several industrial and medical applications including diagnostic ultrasound, sonochemistry, etc. [11]. This equation is solved numerically using the Finite Difference in Time Domain (FDTD) method for the case of a non-isothermal attenuating medium. Various forms of initial disturbances are considered and the steepening of the wave front and the corresponding shock formation distances and times are computed.

2 Westervelt Equation

The Westervelt equation describes the propagation of an acoustic wave in a quiescent medium in the presence of viscous dissipation and nonlinearity effects. In the absence of temperature gradients, simpler equations such as the inviscid Burgers' equation $u_{\mathrm{t}} + cu_{\mathrm{x}} = 0$, where c is the nonlinear sound propagation velocity, can also be employed [7]. However, this equation allows for wave propagation in only one direction. Hence, it is not suitable for studying wave propagations in temperature inhomogeneous mediums wherein the change in the acoustic impedance arising from the variation in temperature reflects a part of the incident wave. The Westervelt equation [6] is written as:

$$\rho_0 \nabla \cdot (\rho_0 \nabla p) + \frac{1}{c_0^2}\frac{\partial^2 p}{\partial t^2} + \frac{\delta}{c_0^4}\frac{\partial^3 p}{\partial t^3} + \frac{\Gamma}{\rho_0 c_0^4}\frac{\partial^2 p^2}{\partial t^2} = 0, \tag{1}$$

where c_0 and ρ_0 are the local sound speed and density of the medium at rest, δ is the dissipation coefficient and Γ, also referred to as the nonlinearity coefficient β in acoustics, is the fundamental derivative of gasdynamics [9]:

$$\Gamma = 1 + \frac{\rho}{c}\left(\frac{\partial c}{\partial \rho}\right)_s \tag{2}$$

The diffusivity coefficient is given by

$$\delta = \frac{1}{\rho_0}\Big(\frac{4}{3}\mu + \mu_B\Big) + \frac{\kappa}{\rho_0}\Big(\frac{1}{c_v} - \frac{1}{c_p}\Big), \tag{3}$$

where μ is the shear viscosity, μ_B is the bulk viscosity, κ is the thermal conductivity and c_p and c_v are the specific heats at constant pressure and volume, respectively [12].

2.1 Numerical Method

Spatial and temporal derivatives in Eq. (1) are approximated with discrete differences using the Finite Difference Time Domain (FDTD) method [5]. The spatial dimension is divided into N_{x} elements with equal spacing of Δx and is indexed with i. Absorbing boundary conditions are implemented at the domain boundaries to prevent numerical reflections from affecting the results. The spatial derivative is computed using second-order accurate, central differences as

$$\frac{\partial^2 p}{\partial x^2} \approx \frac{1}{(\Delta x)^2}\big(p^n_{i+1} - 2p^n_i + p^n_{i-1}\big). \tag{4}$$

The temporal dimension is discretized into N_{t} timesteps with a uniform spacing of Δt and index n. The time derivatives are computed using second-order accurate, central differences with the nonlinear and absorption terms expanded using backward differencing, resulting in

$$\frac{\partial^2 p}{\partial t^2} \approx \frac{1}{(\Delta t)^2}\big(p^{n+1}_i - 2p^n_i + p^{n-1}_i\big), \tag{5a}$$

$$\frac{\partial^3 p}{\partial t^3} \approx \frac{1}{2\Delta t^3}\big(5p^n_i - 18p^{n-1}_i + 24p^{n-2}_i - 14p^{n-3}_i + 3p^{n-4}_i\big), \tag{5b}$$

$$\frac{\partial^2 p^2}{\partial t^2} = 2\Big[\Big(\frac{\partial p}{\partial t}\Big)^2 + p\frac{\partial^2 p}{\partial t^2}\Big] \approx 2\Big[\frac{3p^n_i - 4p^{n-1}_i + p^{n-2}_i}{2\Delta t} + \frac{2p^n_i - 5p^{n-1}_i + 4p^{n-2}_i - p^{n-3}_i}{\Delta t^2}\Big]. \tag{5c}$$

Equations (5) are substituted into Eq. (1) and solved for p^{n+1}_i. Since Eq. (5b) requires five time steps for initialization, the starting waveform is advected using the second-order approximation for nonlinear propagation velocity for $n = 1 \ldots 5$.

Computations are performed in a domain of length 9 m with a uniform grid of 1 mm spatial discretization. The time step of the simulation is chosen to be 1 μs to ensure numerical stability. The source is simulated to be siloxane D_6, a BZT fluid, whose medium temperature and pressure are set at 369 °C and 9 bar respectively. The value of Γ estimated with technical equations of state based on Helmholtz energy [3,8] at this state is –0.15, therefore the flow is theoretically affected by nonclassical gas dynamic conditions. The dimensions of the numerical domain and the initial conditions of the simulation are chosen to match the Flexible Asymmetric Shock Tube (FAST) facility, a shock-tube test setup designed at the Delft University of Technology with the aim of studying the propagation of expansion waves in the NICFD regime [9].

The location at which a shock wave forms is identified by plotting the inverse of the slope of the wave front along the x-direction. Since the shock wave is a discontinuity with the slope of the wave front being infinite, the point at which the inverse of the slope becomes zero provides the shock formation distance [10]. The slope here is expressed as the gradient in the local acoustic velocity $(\partial u/\partial x)$ along the wavefront. To prevent numerical instabilities, the domain is defined to have $\Gamma = 0$ till $0.2 \cdot L_0$ after which Γ is calculated using the thermodynamic model.

3 Results

Figure 1 illustrates a result of simulating the propagation of a right-travelling triangular rarefaction wave of amplitude 50 kPa and wavelength 0.72 m in D_6 with uniform temperature. The nonlinear steepening is shown in Fig. 1 (a) by comparing the waveform of the same initial disturbance which travels in a hypothetical linear medium, and in a non-linear medium. Since the fluid temperature is constant, the value of $(\partial u/\partial x)^{-1}$ is expected to decrease linearly down to zero. Figure 1 (b) illustrates this trend, though calculated values are also affected by a spurious oscillation which is expected to occur when estimating the slope.

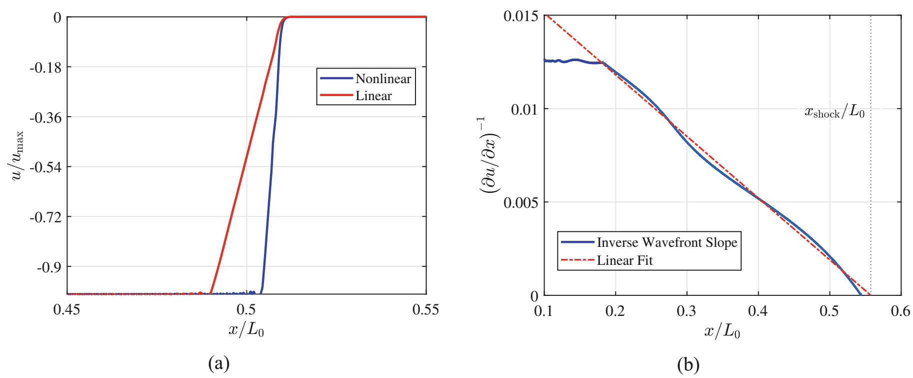

Fig. 1. (a) Nonlinear steepening of a rarefaction wave close to x_{shock} (b) Estimation of $\mathrm{x}_{\text{shock}}$ using the wavefront slope.

The same type of analysis is performed for the case of an inhomogeneous temperature distribution. A sinusoidal variation of 1 °C in temperature about a mean value of 370 °C is assumed and the corresponding values of Γ are computed using the same thermodynamic model. Figure 2(a) shows calculated propagation of the wave front into the medium (left axis) and the variation in Γ along the medium on the right. It can be seen that, unlike what can be noticed in Fig. 1(b), the slope of $(\partial u/\partial x)^{-1}$ is no longer constant as the wave continuously steepens and relaxes as the temperature varies along the medium. Remarkably, the rarefaction steepens to form a shock despite the thermodynamic states of medium display positive Γ in several locations. This observation can be justified by the fact that the bulk of the medium is in the nonlinear thermodynamic region, resulting in the overall effect that the wave steepens into a rarefaction shock wave. The effect of the local linear regions where $\Gamma \simeq 0$ is also visible by the inflection in $(\partial u/\partial x)^{-1}$ curve between the local extrema.

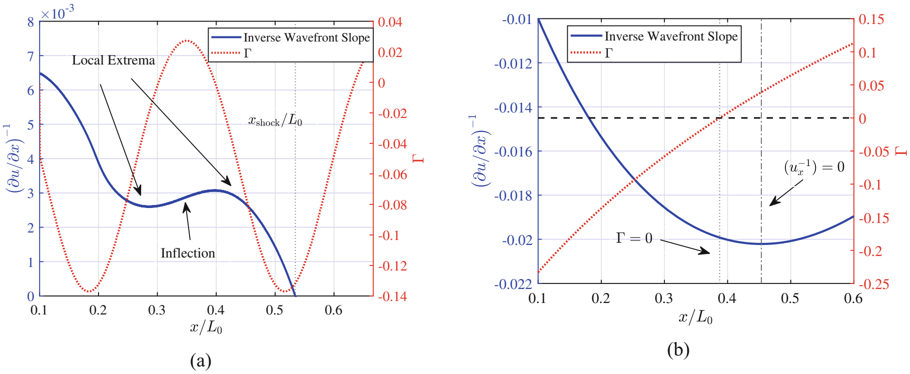

Fig. 2. (a) Steepening of the rarefaction wavefront in D6 with sinusoidally-varying temperature (b) Steepening of the rarefaction wavefront in D6 with linearly-varying temperature—Locations where $\Gamma = 0$ (······) and where $\left[(\partial u/\partial x)^{-1}\right]' = 0$ (- - -)

Another interesting feature can be observed in Fig. 2 at the locations where $\Gamma = 0$. One would expect that the wave would propagate unchanged if $\Gamma = 0$; thus the tangent of $(\partial u/\partial x)^{-1}$ at these locations must also be 0. However, it can be observed that this flattening of the wavefront always succeeds the point where Γ is zero. This can be seen clearly in Fig. 2(b), which shows the propagation of a compression wave in a fluid with temperature increasing linearly from 367.5 °C to 372 °C. Here, it is apparent that the compression initially relaxes into a non-ideal compression fan and steepens as the value of Γ becomes positive.

The vertical lines in Fig. 2(b) represent the axial locations where Γ is zero and where the wavefront starts steepening into a compression shock. It can be clearly observed that in a narrow region right after the point where $\Gamma = 0$, the compression wave continues to relax despite Γ becoming positive, indicating that the variation in the sound speed and density in this region has a significant influence on the wave distortion. Except in this region, the sign and magnitude of Γ remain the most important characteristics governing the nature of the nonlinear distortion of the wave.

4 Conclusions and Future Work

Preliminary results of a numerical investigation on the nonclassical propagation of nonlinear waves in case the medium is affected by temperature variations at the boundary of the domain indicate that, though the amplitude of the initial disturbance is crucial for nonlinear steepening, the minimum amplitude for shock formation is strongly dependent on the temperature distribution, and therefore, the variation of the fundamental derivative in the medium. Though Γ is the most important parameter influencing shock formation, it is observed that rarefaction shocks can steepen even in regions of positive nonlinearity before transitioning into a rarefaction fan. This study resulted in a tool that allows computing shock parameters such as formation distance and time for the case of a medium affected by varying temperatures. Further sensitivity studies will be performed to analyse the effect of temperature inhomogeneities on nonlinear wave propagation and shock formation. In addition, the applicability of this analysis to industrial problems will be explored.

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