ORIGINAL PAPER



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Shock discontinuities: from classical to non-classical shocks

This paper is dedicated to the memory of Franz Ziegler

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Abstract The possibility of shocks was first suggested by Stokes in 1848, but no consistent theory emerged for another almost 30 years. Indeed, severe criticism by Lord Kelvin and Lord Rayleigh led him to finally discard this idea. In the meantime, algebraic shock conditions had been derived by Rankine and Hugoniot, and their names have come to be associated with the shock conditions generally. As Thompson (Compressible-fluid dynamics, McGraw-Hill, New York, 1972) concludes, "Stokes's claim to recognition for his discovery has been diverted by circumstance." Starting with a brief discussion of these early developments, the present review paper will then concentrate on the important question of how to select from all formally possible solutions of the so-called admissibility problem. Of course, a necessary condition is provided by the second law of thermodynamics which states that the entropy must not decrease during adiabatic changes of state. For perfect gases, this requirement is also a sufficient condition to rule out "impossible" shocks. For fluids with an arbitrary equation of state and/or situations where in addition to thermoviscous effects, dispersive effects also come into play this is not the case in general. The selection of physically admissible solutions is then found to be a more delicate matter and may result in new types of shocks which differ distinctively from their classical counterparts and, therefore, are termed non-classical shocks.

Mathematics Subject Classification 76Lxx · 76Nxx

1 Introduction

Early mechanics evolved parallel to the theory of differentiation. Quantities of interest—e.g., the position of planets in the solar system—were taken to be described by smooth functions governed by differential equations or systems of differential equations. Therefore, the first question to be addressed in this paper is: What kindled the idea that differential equations or systems of differential equations alone might be incomplete in general to provide solutions of problems arising in mechanics and in particular in the continuum theory of fluid mechanics and thus have to be supplemented with an additional set of equations now known as jump conditions which determine the motion of surfaces of discontinuities we refer to as shock discontinuities or simply shocks?

Before I try to answer this question, let us have a brief look at three examples of real shocks. Figure 1 shows photographs of shocks generated by imploding cavitation bubbles in water at different times after the collapse, Lauterborn and Kurz [39]. With increasing time, shocks, visualized by thin black lines, are seen to move away from their point of origin. Here a typical length scale is of the order of 10^{-2} m. Bigger shocks are generated

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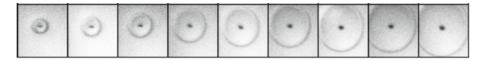


Fig. 1 Photographic series of the dynamics of a laser produced bubble collapse in water. The bubble reaches its maximum diameter of $1.1 \text{ mm } 99.5 \,\mu\text{s}$ before the first frame



Fig. 2 The first explosion of a nuclear weapon on July 16, 1945: 16 ms after ignition. Photo: National Archives, Washington, D.C



Fig. 3 Spiral Galaxy M81. Photo: NASA

by explosions and in particular explosions of nuclear bombs as evidenced by Fig. 2 which documents the first test of such a bomb on July 16, 1945. Here the typical length scale is of the order of 10^3 m. As a final example, Fig. 3 shows an astronomic photography of the spiral galaxy M81. This galaxy exhibits two arms, and as in other galaxies of this type, these arms are thought to be accompanied by shocks which heat the interstellar gas, initiate the formation of new stars and extend over thousands of light years. The size of shock waves in our universe, therefore, covers at least 10^{21} orders of magnitude which clearly underlines the importance of the question formulated at the beginning of this section: How did theory pave the way to our current understanding of this phenomenon?

2 Early history

An important first step was taken by Poisson. In 1808 he published the celebrated result

$$w = f(x - (w + a)t) \tag{1}$$

for the distribution of the fluid velocity inside an acoustic wave of finite amplitude which propagates to the right, Fig. 4. Here a, x, t and w denote, respectively, the speed of sound, the propagation distance, the time and the fluid velocity, while the function f specifies the wave profile at t = 0. As in Newton's theory of infinitesimally

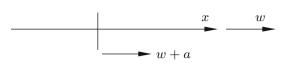


Fig. 4 One-dimensional right-running acoustic wave

small disturbances, Poisson assumes that the propagation process is isothermal so that a remains constant. The convected sound speed a + w, however, depends on the fluid velocity and thus causes the wave profile to distort with increasing propagation distance x: Parts of the wave where w is smaller than in the unperturbed quiescent state will flatten out while regions of increased fluid velocity will steepen. But because such a result had never been observed experimentally, he nevertheless concludes "... that the original disturbance is transmitted uniformly with a speed equal to a, ..." and missed the importance of his result.

Forty years later, Challis [4], commenting on Airy's remark on his theories of sound, finds (obviously not knowing Poisson's previous work) that "the velocity of propagation is different from the sound velocity and certain faster parts in the wave profile will take over slower ones, thus leading to ambiguous mathematical solutions", (Challis paradox).

In the same year Stokes [64] concludes that ambiguous mathematical solutions occur if Poisson's formula is applied at distances larger than x_s where the velocity profile first exhibits a vertical tangent, i.e., beyond its range of validity. He then states: "Of course, after the instant at which expression A (for the slope of the wave profile) becomes infinite, some other motion will go on ... Perhaps the most natural supposition to make for trial is, that a surface of discontinuity is formed, in passing across which there is an abrupt change of density and velocity. The existence of such a surface will presently be shown to be possible ...," but unfortunately no follow-up paper from his pen was published during the next 30 years.

Ten years later Earnshaw [10] presents his theory of sound waves of finite amplitude. His results are of exactly the same form as derived by Poisson, but he recognizes that the wave propagation process is adiabatic rather than isothermal so that the sound speed does not remain constant. Also, in contrast to Poisson, he accepts the fact that the wave profile distorts with increasing propagation distance and, as Stokes, considers the possibility of a discontinuity forming. But then he concludes: "As, however, discontinuity of pressure is a physical impossibility, it is certain Nature has a way of avoiding its actual occurrence."

Without doubt the paper¹ "Über die Fortpflanzung ebener Luftwellen von endlicher Schwingungsweite" published by Riemann [55] is the milestone contribution to the history of shock waves. As Earnshaw he recognizes that the wave propagation process is adiabatic. Also, by utilizing Monge's method of characteristics, he not only derives formulas for right *or* left running waves but also for interacting right *and* left running waves. Most important, he shows that shocks form naturally inside compression waves. In his own words²: "Die Verdichtungswellen, d.h. Theile der Wellen, in welchen die Dichtigkeit in Fortpflanzungsrichtung abnimmt, werden demnach bei ihrem Fortschreiten immer schmäler und gehen schließlich in Verdichtungsstöße über". He then concludes³: "Durch die vollständige Lösung dieser Aufgabe (the initial value problem) dürften die vor einiger Zeit zwischen den Englischen Mathematikern Challis, Airy und Stokes lebhaften Fragen ... zu klarer Entscheidung gebracht worden sein". But as turned out this was not the case.

In 1877 Stokes received a letter by his former student Lord Rayleigh, who at this time was preparing the publication of his book Theory of Sound:

Dear Prof. Stokes,

In consequence of our conversation the other evening I have been looking at your paper "On a difficulty in the theory of sound," Phil. Mag. Nov. 1848. The latter half of the paper appears to me liable to an objection, as to which (if you have time to look at the matter) I should be glad to hear your opinion ... (there follows a "proof"). It would appear therefore that on the hypotheses made, no discontinuous change is possible. I have put the matter very shortly, but I dare say what I have said will be intelligible to you.

¹ "On the propagation of planar waves of finite amplitudes in air".

 $^{^2}$ "The compression waves, i.e., those parts of the wave in which the density increases in propagation direction, therefore decrease in length and finally evolve into compression shocks".

³ "Through the complete solution of this problem (the initial value problem) questions which some time ago were discussed lively between the English mathematicians Challis, Airy, and Stokes appear to be brought to a clear solution".

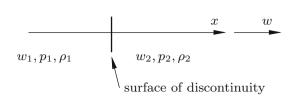


Fig. 5 Shock discontinuity in steady one-dimensional flow

Stokes replied at once:

Dear Lord Rayleigh,

Thank you for pointing out the objection to the queer kind of motion I contemplated in the paper you refer to. Sir W. Thomson pointed the same out to me many years ago, and I should have mentioned it if I had had the occasion to write anything bearing on the subject, or, without that, my paper had attracted attention. It seemed, however, hardly worthwhile to write a criticism on a passage in a paper which was buried among other scientific antiquities.

P.S. You will observe I wrote somewhat doubtfully about the possibility of the queer motion.⁴

For Rayleigh this apparently settled the matter. The following passage appears in his Theory of Sound ([54]; vol. 2, p. 40): but it would be improper to pass over in silence an error on the subject of discontinuous motion into which Riemann and other writers have fallen. It has been held that a state of motion is possible in which the fluid is divided into two parts by a surface of discontinuity.

3 Shock jump relationships established!

Obviously not noticed by the disagreeing parties almost 25 years earlier, algebraic shock conditions had already been derived by the Scottish engineer Rankine [53] and the French professor of mechanics Hugoniot [15, 16], assuming one-dimensional steady flow as sketched in Fig. 5 where w, p, ρ and h denote the fluid velocity, the pressure, the fluid density and the specific enthalpy. Subscripts 1 and 2 specify values immediately upstream and downstream of the surface of discontinuity. The balances of mass, momentum, and energy in integral rather than differential form then lead to the results summarized below:

mass:
$$\rho w = \text{const} \Rightarrow \rho_2 w_2 = \rho_1 w_1,$$
 (2)

momentum:
$$\rho w^2 + p = \text{const} \implies \rho_2 w_2^2 + p_2 = \rho_1 w_1^2 + p_1,$$
 (3)

energy:
$$w^2/2 + h = \text{const} \Rightarrow w_2^2/2 + h_2 = w_1^2/2 + h_1.$$
 (4)

Taking the upstream state to be known, these balances provide three equations for the four unknowns w_2 , p_2 , ρ_2 and h_2 . Therefore, an additional relationship, the caloric equation of state,

$$h = h(p, \rho),\tag{5}$$

which specifies h in terms of p and ρ is required to close the system.

At first sight the assumption of one-dimensional steady flow imposed before might appear overly restrictive. But taking into account that shock discontinuities do not contain mass and represent localized phenomena it is easily seen that the associated relationships are neither affected by inertia nor by curvature effects. Therefore, they can always cast into this canonical form which will be taken as the basis for further considerations.

An important result is obtained by the elimination of the fluid velocity w from the energy balance. This leads to the Rankine–Hugoniot relationship

$$[h] = [p](v_1 + v_2)/2, \quad v = 1/\rho, \tag{6}$$

where v is the specific volume and square brackets denote the jump of any physical quantity $q: [q] = q_2 - q_1$.

⁴ This correspondence cited by Thompson [69], pp. 311–312, is taken from Truesdell's preface to Stokes' collected "Mathematical and Physical papers" 1, Johnson Reprint, New York, 1966. Readers interested in more biographical information concerning pioneers involved in the development of the theory of shocks are referred to Johnson and Chéret [17], Salas [56].

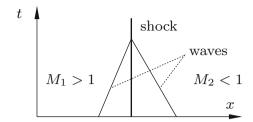


Fig. 6 Shock formation through intersecting wave fronts

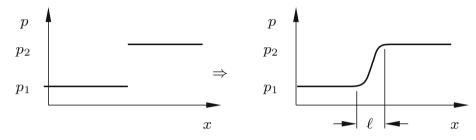


Fig. 7 Existence of an internal (thermoviscous) shock structure

Equation (6) has the advantage that it only contains thermodynamic quantities and thus holds for arbitrary fluids. Specific fluid properties enter via the caloric equation of state and when combined with the Rankine–Hugoniot relationship results in the so-called shock adiabat

$$p_2 = f(p_1, v_1; v_2). \tag{7}$$

If one specifies values p_1 , v_1 upstream of the shock and v_2 downstream of the shock, then the formal solution of the shock adiabat yields the downstream pressure p_2 . But then the question arises: Are all formal solutions also physically realizable solutions and if the answer is no the question is how to select from all formal solutions those which are physically realizable solutions? This is the so-called admissibility problem.

4 Shock admissibility

Of course a necessary condition for the existence of shocks is provided by the second law of thermodynamics which states that the specific entropy s must not decrease during adiabatic changes of state, Jouget [18, 19], Zemplén [76, 77]:

$$[s] \ge 0. \tag{8}$$

A second natural requirement is that shocks must be able to form inside the fluid. The only known mechanism of shock formation is by intersecting wave fronts—or in more mathematical terms—by intersecting characteristics, Becker [1], Fig. 6. When expressed in terms of the local Mach number M = w/a, one thus obtains the wave speed ordering relationship which states that M has to be larger/smaller than 1 upstream/downstream of the shock:

$$M_1 > 1 > M_2.$$
 (9)

Finally it should be noted that the derivation of the shock jump relationships was based on the assumption, not mentioned explicitly so far, that the effect of viscous stresses and heat fluxes is negligible. By taking these effects into account, one expects that discontinuities predicted by the shock jump relationships are replaced by smooth profiles as sketched in Fig. 7 for a compression shock moving to the right. A more stringent criterion than (8) and (9), therefore, is that realizable shocks admit thermoviscous profiles, Prandtl [50]. Obviously, such an approach reduces the idea to treat shocks as discontinuities in order to obtain information how the upstream and downstream states are connected without the need to investigate in detail the flow behavior inside such "shock layers" taken to be thin on a global length scale where gradients otherwise negligible are large enough to generate significant viscous stresses and heat fluxes.

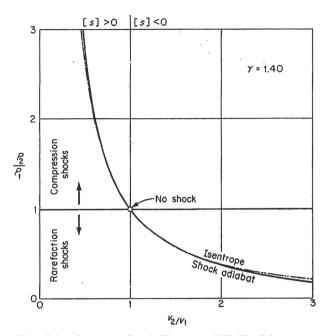


Fig. 8 Shock adiabat and reversible adiabat (isentrope) for air, Thompson [69], Fig. 7.9

5 Shock admissibility in perfect gases

Before proceeding further, we will briefly consider the most simple case of perfect gases. Then the combination of the Rankine–Hugoniot relationship (6) with the caloric equation of state

$$h = c_{\rm p}T + {\rm const} = \frac{\gamma}{\gamma - 1} pv + {\rm const}, \quad \gamma = \frac{c_{\rm p}}{c_{\rm v}} > 1,$$
 (10)

where c_v and c_p denote, respectively, the specific heats at constant volume and constant pressure, yields this analytical result for the shock adiabat, von Kármán [72]:

$$\frac{[p]}{[\rho]} = \gamma \, \frac{p_2 + p_1}{\rho_2 + \rho_1}.\tag{11}$$

Here *T* denotes the absolute temperature and γ is the ratio of the specific heats at constant pressure and constant volume. As a specific example, Fig. 8 displays the shock adiabat for air, $\gamma = 1.4$, in the p_2/p_1 , v_2/v_1 diagram. Also included in this diagram is the reversible adiabat, the isentrope. One immediately recognizes that the entropy jump is positive for compression shocks $v_2/v_1 < 1$ and negative for rarefaction shocks $v_2/v_1 > 1$. Therefore, for $\gamma = 1.4$, compression shocks are admissible while rarefaction shocks are inadmissible. Rigorous mathematical proofs that this is true for all perfect gases have been given by Jouget [18,19] and Zemplén [76,77]. The conclusion that rarefaction shocks are impossible in perfect gases has entered the literature as the Zemplén theorem, unfortunately sometimes without mentioning the basic assumption that the fluid is a perfect gase.

The next step toward a deeper understanding of the nature of shocks was taken by Becker [1] who showed in his Habilitationsschrift "Stoßwelle und Detonation" that for perfect gases the admissibility requirements following from the second law of thermodynamics (8) and the wave speed requirement (9) are equivalent; in other words: All shock discontinuities which can form mechanically by coalescing characteristics automatically satisfy the second law of thermodynamics. In my opinion this is one of the most "beautiful" results in the theory of shocks and expressed equally "beautifully" by the relationship due to Prandtl

$$w_1 w_2 = a^{*2}, (12)$$

where a^* is the critical sound speed, i.e., the value of a at M = 1, computed under the assumption of constant entropy and total enthalpy.

Finally let us turn to the third admissibility criterion, the existence of a continuous shock profile. That such shock profiles exist has been shown first by Prandtl [50] and Taylor [67], see Sect. 7. So we conclude that for perfect gases all three admissibility criteria are equivalent.

6 Admissibility in arbitrary fluids

Shocks in arbitrary fluids were investigated first by Duhem [9]. Concentrating on weak shocks he showed that the first and second derivative of the specific entropy *s* with respect to ρ along the shock adiabat and evaluated at the upstream state vanish. He also demonstrated that the third derivative of *s* with respect to ρ , again evaluated at the upstream state, can be expressed in terms of a function $H(p, \rho)$:

$$\left(\frac{\partial^3 \Sigma}{\partial \rho_2^3}\right)_{\rho_2 = \rho_1} = \frac{1}{2\rho_1^3 T_1} H(p_1, \rho_1), \quad H(p_1, \rho_1) = \left(2\frac{\partial \Pi}{\partial \rho_2} + \rho_2 \frac{\partial^2 \Pi}{\partial \rho_2^2}\right)_{\rho_2 = \rho_1}$$
(13)

where

$$s_2 = \Sigma(\rho_2; p_1, \rho_1), \quad p_2 = \Pi(\rho_2; p_1, \rho_1).$$
 (14)

Here functions Σ , Π specify values s_2 , p_2 in terms of ρ_2 for a given upstream state $\rho = \rho_1$, $p = p_1$. Consequently, the entropy jump across weak shocks in arbitrary fluids is proportional to $H(p_1, \rho_1)$ and the third power of [v]:

$$[s] = -\frac{v_1^3}{12T_1} H(p_1, v_1) [v]^3 + \cdots .$$
(15)

Duhem thus concludes that "if the quantity H is positive, the region that is upstream from the wave is the one where the fluid is denser; it is the region where the fluid is less dense that is upstream from the wave when H is negative. In the first case we say that the shock propagates a condensation, and in the second case, it propagates an expansion".

It is easily shown that H can also be expressed in the form

$$H(p_1, v_1) = v_1^3 \left(\frac{\partial^2 p}{\partial v^2}\right)_{s=s_1}$$
(16)

first published by Bethe [3] who apparently was unaware of Duhem's work which preceded his own by almost 40 years. The significance of this result derives from the fact that it relates the entropy jump directly to the curvature of isentropes in the p, v diagram. The admissibility requirement following from the second law of thermodynamics, therefore, can easily be checked by looking at the shape of isentropes in this diagram. If they are curved up as in the case of perfect gases, weak shocks are compression shocks, while they are rarefaction shocks if isentropes are curved down. In the more recent literature, one usually introduces the non-dimensional measure of the curvature of isentropes

$$\Gamma = \frac{v^3}{2a^2} \left(\frac{\partial^2 p}{\partial v^2}\right)_s = \frac{1}{a} \left(\frac{\partial \rho a}{\partial \rho}\right)_s \tag{17}$$

which plays an important role in many areas of compressible fluid dynamics and, following a proposal by Thompson [68], is called the fundamental derivative of gas dynamics. For example, the equivalent expression of Γ in Eq. (17) which involves the derivative of the speed of sound with respect to the fluid density already indicates its importance for the treatment of acoustic waves in general fluids. Indeed it is easily shown that the change of the convected sound speed σ with fluid density in right or left running waves is proportional to Γ :

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\rho}\right)_{s} = \pm \frac{a}{\rho} \Gamma, \quad \sigma = w \pm a.$$
(18)

Therefore, the sign of Γ and thus the curvature of isentropes in the *p*, *v* diagram decides whether compressive or expansive waves steepen as pointed out first by Becker [1]. In his Habilitationsschrift mentioned before, he writes⁵: "In einem gegebenen Medium können mechanisch nur Versdichtungsstöße oder Verdünnungsstöße

⁵ "In a given medium only compression or rarefaction shocks can form mechanically if $(\partial^2 p / \partial v^2)_s$ is positive or negative".

entstehen je nachdem ob $(\partial^2 p / \partial v^2)_s$ positiv oder negativ ist". Also he adds⁶: "Genau dieses Kriterium wird uns später (Sect. 6) bei der Betrachtung der thermodynamischen Möglichkeiten wieder begegnen."

These "Möglichkeiten" have been studied in more detail almost 20 years later by Bethe [3]. His classified report "The theory of Shock Waves for an Arbitrary Equation of State" was part of the Manhattan project to build a nuclear bomb which generates extremely intensive shocks where gases no longer behave as perfect gases. Assuming that the pressure p is a unique function of v, T or equivalently of s, v

$$p = p(v, T) = p(s, v) \tag{19}$$

he—obviously unaware of Becker's achievements—states: "We shall find that certain assumptions I: $(\partial^2 p / \partial v^2)_s > 0$, II: $v (\partial p / \partial u)_v > -2$, III: $(\partial p / \partial v)_u < 0$ where *u* denotes the specific internal energy must be made concerning the equations of state in order to prove the existence and uniqueness of Hugoniot's shock wave equations. The most important of these conditions is

$$(\partial^2 p / \partial v^2)_s > 0. \tag{20}$$

Since $(\partial p/\partial v)_s$ is the adiabatic compression modulus, condition (20), means that this modulus must increase with increasing compression. Condition (20) is very plausible; It will be shown that for all single-phase systems the condition is very well satisfied." He then adds: "Analysis shows that none of the three conditions I, II, III is required by any general thermodynamic or statistical argument because it can be shown that that for each of the three conditions there exist some substances for which the condition is violated at certain temperatures and densities." In short, the existence or nonexistence of rarefaction shocks is not a consequence of thermodynamic reasoning but a consequence derived solely from constitutive relations. Taking these to be the thermal and caloric equations of state of the form, where c_v is the specific heat at constant volume,

$$c_{\rm v} = c_{\rm v}(v, T),\tag{21}$$

Bethe derives the key result

$$\left(\frac{\partial^2 p}{\partial v^2}\right)_s = \underbrace{\frac{\partial^2 p}{\partial v^2}}_{(d)} - \underbrace{\frac{3T}{c_v} \frac{\partial p}{\partial T} \frac{\partial^2 p}{\partial v \partial T}}_{(c)} + \underbrace{\frac{3T}{c_v^2} \left[\frac{\partial^2 p}{\partial T^2}\right]^2 \frac{\partial c_v}{\partial v}}_{(b)} + \underbrace{\frac{T}{c_v^2} \left[\frac{\partial p}{\partial T}\right]^3 \left[1 - \frac{T}{c_v} \frac{\partial c_v}{\partial T}\right]}_{(a)}$$
(22)

and concludes: "From Eq. (22) we can easily get an idea about the terms which might theoretically cause $(\partial^2 p / \partial v^2)_s$ to be negative." He rapidly dismisses that the terms (a), (b) and (c) may cause the curvature of isentropes to become negative and turns to the first term (d). He points out that "this term may be negative. This happens at and near the critical temperature for volumes greater than the critical volume. In this case the second term (c) more than outweighs the first." To support this conclusion Bethe investigates van der Waals gases with constant c_v

$$p = \frac{RT}{v-b} - \frac{\alpha}{v^2}, \quad c_v = \text{const.}$$
(23)

He finds that the adiabatic derivative $(\partial^2 p / \partial v^2)_s$ can be negative only for

$$\beta = \frac{c_{\rm v}}{R} > 17.5. \tag{24}$$

Here *R* denotes the universal gas constant. The same conclusion was reached later by Zel'dovich [75]. But Bethe obviously dismisses this possibility when he writes: "Such a large value (of β) is practically impossible for any gas at a temperature as low as the critical temperature where values of β between 2.5 and 4 are the rule. We find therefore that $(\partial^2 p / \partial v^2)_s$ remains positive near the critical point for all real gases obeying the van der Waals equation."

This settled the question for the next 30 years. But in 1971 this point of view was contested by Thompson in a paper in which he discussed the role of Γ in the theory of shocks. Also by taking into account more recent information concerning fluids which consist of complex molecules and making use of more sophisticated equations of state Thompson and Lambrakis [69] were able to demonstrate the existence of negative Γ fluids and thus also the possible existence of negative shocks, i.e., rarefaction shocks. Honoring the pioneering works

⁶ "Exactly this criterion will be encountered later (Sect. 6) by consideration of the thermodynamic possibilities".

by Bethe, Zel'dovich and Thompson negative Γ fluids are now commonly summarized as Bethe–Zel'dovich– Thompson fluids or in short as BZT fluids following a proposal by Cramer in the early 1980s.

Interestingly the existence of negative Γ fluids is suggested already by theoretical reasoning independent of any assumptions about specific forms of equations of state, Kluwick [25]. According to the phenomenological theory of thermodynamics, the dependence of the specific internal energy u and the specific entropy s on v and T is equally important for gases of low molecular complexity where $\beta = O(1)$. However, for gases of moderate and large molecular complexity β is large compared to 1 and both u and s depend mainly on T with small corrections due to variations of v accounted for by functions f and g that reflect the specific properties of the equations of state:

$$u(v,T) = \Phi(T) + (1/\beta)f(v,T), \quad s(v,T) = \Psi(T) + (1/\beta)g(v,T).$$
(25)

Substitution into the Rankine–Hugoniot relationship then yields the result that temperature jumps caused by shock discontinuities are small and of the order of $1/\beta$:

$$[T]/T_1 = O(1/\beta).$$
(26)

As a consequence shock adiabats, isotherms and isentropes almost collapse into a single curve in the p, v diagram. Therefore, in the definition (17) derivatives at constant s can approximately be replaced by derivatives at constant T:

$$\Gamma = \frac{v^3}{2a^2} \left(\frac{\partial^2 p}{\partial v^2}\right)_s = \frac{v^3}{2a^2} \left(\frac{\partial^2 p}{\partial v^2}\right)_T + O(1/\beta)$$
(27)

and since isotherms are known to have negative curvature in the general neighborhood of the thermodynamic critical point Γ is expected to be negative there too. Therefore, gases with moderate and large molecular complexity are candidates of BZT fluids. This raises the question: why bother with fluids so "exotic" as BZT fluids?

- Of course one reason is that the existence of rarefaction shocks is of fundamental theoretical interest but there are also a number of practical applications, e.g., Organic Rankine Cycles; see, e.g., Kluwick [23], where the use of BZT fluids might be advantageous.
- Due to the fact that isentropes and shock adiabats differ only slightly in the *p*, *v* diagram shock losses are in general smaller than in perfect gases and other gases of low molecular complexity which might be used to improve efficiency of turbomachines.
- Rarefaction shocks accelerate rather than decelerate the fluid and there is no danger of flow separation if they interact with boundary layers.
- Also, it is found that the lower critical Mach number which limits the regime of shock-free flow expands substantially, and this again is expected to improve the performance of turbomachines using BZT fluids as working fluids.

For the treatment of shocks in such fluids, it is essential to acknowledge the qualitative changes of the shock adiabat associated with increasing values of β , Fig. 9. If β is of order one, shock adiabats are curved up as in the case of perfect gases. For large values of β , however, shock adiabats exhibit two inflexion points separating a bulge where the curvature is negative similar to isotherms in the general neighborhood of the thermodynamic critical point. To simplify the analysis of shock behavior we make use of the relationship

$$\frac{[p]}{[v]} = -\rho_1^2 w_1^2 = -\rho_2^2 w_2^2 \tag{28}$$

which follows directly from the shock jump conditions. It relates the slope of the straight line connecting the upstream and downstream states on the shock adiabat with the square of the associated mass fluxes. In the western world, this line is called the Raleigh line referring to his work on aerial shock waves, Rayleigh [65], but the expression (28) was derived earlier by Mikhel'son [43] and Schuster [62].

For the following two properties of the Rayleigh line are of importance. First, it can be shown, see, e.g., Kluwick [25], that the wave speed ordering relationship is satisfied only if the Rayleigh line does not cut the shock adiabat in interior points. Therefore, a shock with upstream and downstream values of the pressure p_1 and p_2 is admissible while shocks having higher values of the downstream pressure are inadmissible, Fig. 10. Second, it can be shown that if the Rayleigh line is tangent to the shock adiabat in some point, then the Mach number associated with this flow state is equal to one, and the entropy distribution along the shock adiabat

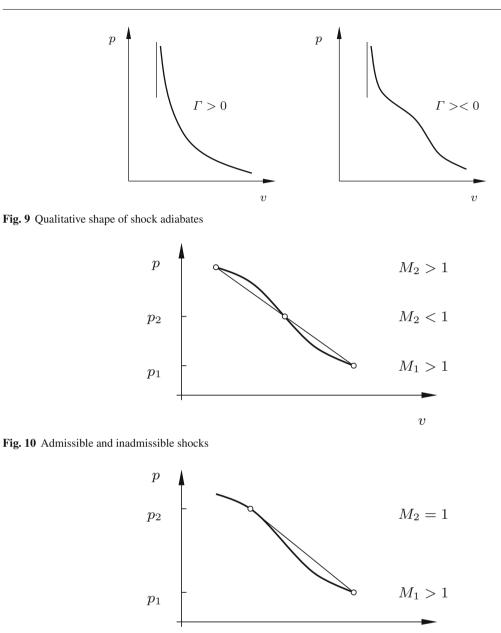


Fig. 11 Sonic shock

exhibits an extremum, Fig. 11. These results motivated Lax [38] and Oleinik [47] to propose the extended wave speed ordering relationship

$$M_1 \ge 1 \ge M_2$$
 if $\left(\frac{\mathrm{d}p}{\mathrm{d}v}\right)_1 \ge \frac{[p]}{[v]} \ge \left(\frac{\mathrm{d}p}{\mathrm{d}v}\right)_2$ (29)

v

which allows the existence of non-classical shocks with Mach number 1 upstream or downstream (sonic shocks) or even with Mach number 1 upstream and downstream (double sonic shocks). Representative examples are shown in Fig. 12.

First let us consider compression shocks with an upstream state 1. Shocks leading to a downstream state 2 are clearly admissible as the Rayleigh line lies above the shock adiabat and the wave speed ordering relationship is satisfied as seen in the x, t-diagram. By increasing the shock strength one approaches state 3 where the

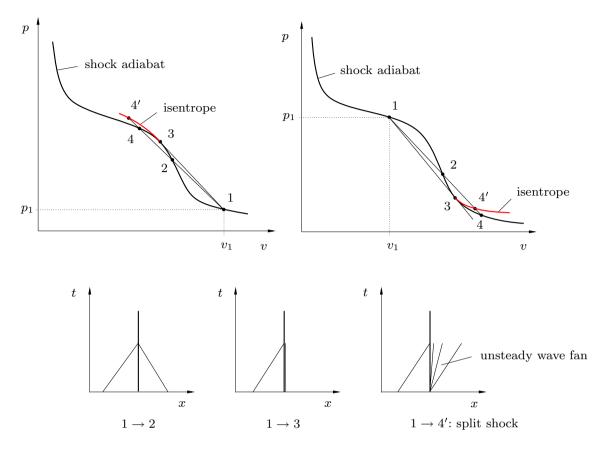


Fig. 12 Admissible and inadmissible compression/rarefaction shocks

Rayleigh line is tangential to the shock adiabat indicating that a sonic downstream state has been reached: in the x, t-diagram the shock front coincides with the wave front downstream of the shock. Also it is clear that single shocks of even higher strength leading for example from state 1 to state 4 are inadmissible as the associated Rayleigh line then cuts the shock adiabat so that the wave speed ordering relationship is violated. By imposing a larger pressure increase, one obtains the x, t-diagram shown on the right: The shock from 1 to 3 having a sonic downstream state is followed by a continuous compression of the fluid along the isentrope starting in point 3 which generates a compression wave fan in the space, time-diagram. Such a compression wave fan is impossible in perfect gases and represents another non-classical feature of BZT fluids. The resulting compound structure which consists of a sonic shock and an attached wave fan is termed a mixed (composite) wave or more specifically a compression split shock. This reveals a further advantage of BZT fluids for practical applications: the limitation of the maximum possible shock strength.

The p, v-diagram on the right-hand side of Fig. 12 indicates that the scenarios resulting from the consideration of rarefaction shocks of varying strength are analogous to those obtained for compression shocks. By increasing the shock strength, i.e., by lowering the downstream pressure, a sonic downstream state is reached eventually. Further decrease in the downstream pressure is possible only through a rarefaction split shock, the combination of a sonic rarefaction shock and an attached expansion wave fan.

As pointed out before (in connection with the discussion of Figs. 10, 11), the entropy distribution on shock adiabats exhibit extrema at sonic points. For compression shocks discussed just before, this implies that *s* increases with increasing values of *p* and reaches a local maximum at the sonic point 3, Fig. 13. Therefore, *s* will still be larger than s_1 for some values p_4 larger than p_3 where the Rayleigh line intersects the shock adiabat so that the wave speed ordering relationship is violated. We thus conclude that the admissibility criteria following from the wave speed ordering relationship and the second law of thermodynamics are no longer equivalent as in the case of perfect gases. As a consequence the requirement of a nonnegative entropy jump is not sufficient in general to rule out inadmissibile shocks. This finding quite naturally leads us to the question concerning the role of the third admissibility requirement formulated in Sect. 4: the existence of a smooth

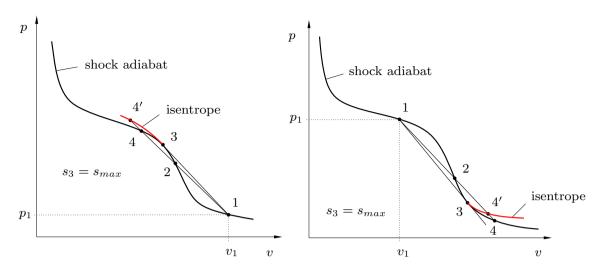


Fig. 13 Comparison of the admissibility criteria following from the second law of thermodynamics and the wave speed ordering relationship

internal dissipative shock structure. Before turning to this problem, let me close the treatment of shocks as surfaces of discontinuity by citing a passage in the paper "The History of Shock Waves" by Kehls [21]: "The puzzling shock wave, characterized by a stepped wave front, was difficult to accept by early naturalists because it involved the abandonment of the principle Natura non facit saltus, ... Surprisingly, however, the problem was successfully tackled neither by experimentalists nor by philosophers but rather by mathematical physicists. Jouget wrote: the shock wave represents a phenomenon of rare peculiarity such that it has been uncovered by the pen of mathematicians, first by Riemann, then by Hugoniot. The experiments followed afterward." In contrast, experimental observation played a decisive role in triggering early investigations which dealt with the internal structure of shocks.

7 Shock structure

In 1903 Stodola published his famous book on steam turbines "Die Dampfturbinen und die Aussichten der Wärmekraftmaschinen" which contains the first studies of the flow characteristics through a supersonic (Laval) nozzle, Fig. 14. He measures the pressure distribution along the nozzle axis and, noticing a sequence of steep pressure increases, states: "I see in these extraordinary violent increases of pressure a realization of the compression shock derived by Riemann". Stodola's results raised Prandtl's interest in this phenomenon and in consequence lead to the first systematic studies of shocks both experimentally and theoretically. Without doubt these studies convinced Prandtl that shocks exist which at that time, as was pointed out before, was still a source of controversy. But Prandtl also recognized that for a deeper understanding of the nature of shock waves, it was necessary to go beyond the theory of jump relationships where shocks were treated as surfaces of discontinuities. In his own words⁷: "Der Unstetigkeit, die sich aus der Theorie ergibt, entspräche nur dann eine physikalische Unstetigkeit, wenn die Reibung und Wärmeleitung im Gas oder Dampf gleich Null wäre; in Wirklichkeit sind diese beiden Größen zwar sehr klein aber endlich. Eine verfeinerte Theorie hat hier anzusetzen". In pursuit of this "program" Prandtl [50] publishes his paper "Zur Theorie des Verdichtungsstoßes". Although less well known than other works from his pen, it must be considered a milestone in fluid mechanics which demonstrates his astounding ability to achieve important physical insight with a minimum of mathematical effort. First he recognizes that in order to capture the essential features of the dissipative shock structure it is sufficient to take into account the effect of heat conduction only and to neglect the effect of viscous stresses. He then proceeds in three steps. Utilizing the energy balance he shows that the heat flux q can be expressed in the form

$$q = \frac{v_1^2}{2w_1^2} \frac{\gamma + 1}{\gamma - 1} (p - p_1)(p_2 - p).$$
(30)

⁷ "The discontinuity following from theory would represent a physical discontinuity only if internal friction and heat conduction in the gas or vapor vanish; in reality these quantities are small but finite. A more refined theory has to start from here."

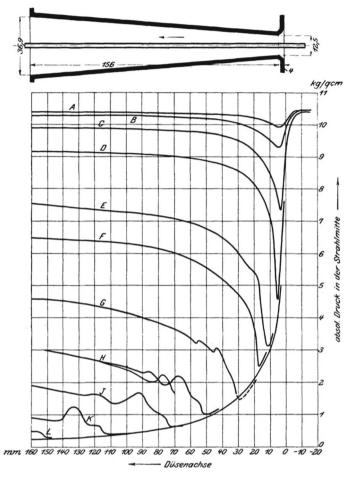


Fig. 14 Pressure distribution in a Laval nozzle, Stodola [63]. The flow is from right to left; the x and y labels specify the distance from the nozzle entry and the pressure at the nozzle axis

A second relationship for q is obtained from Fourier's law of heat conduction

$$q = \frac{\lambda v_1}{w_1} \frac{\mathrm{d}T}{\mathrm{d}x}.$$
(31)

Equating both relationships and taking into account that for weak shocks changes of the temperature are approximately proportional to changes of pressure, i.e., $dT = (v_1/c_p)dp$, he finally obtains the structure equation

$$\delta \frac{dp}{dx} = (p - p_1)(p_2 - p_1), \quad \delta = \frac{\gamma - 1}{\gamma + 1} \frac{2w_1\lambda}{c_p}.$$
 (32)

This equation can be solved quite easily and the general form of the shock profile is shown in Fig. 15. Even more important, the structure equation allows to estimate the shock thickness ℓ . To this end Prandtl approximates the actual profile by its tangent at the inflexion point. The resulting expression

$$\ell = \frac{8(\gamma - 1)\lambda w_1}{(\gamma + 1)c_p} \frac{1}{p_2 - p_1}$$
(33)

leads to the remarkable conclusion that ℓ decreases with increasing shock strength. Specific examples for air at $p_1 = 1$ bar, $T_1 = 0$ °C are summarized in Table 1. For a pressure jump of 0.2 bar ℓ is of the order of 10^{-5} mm, i.e., of the order of the mean free path which indicates that the continuum theory has been stretched up to and perhaps beyond its limits. Weaker shocks generated for example by the supersonic aircraft Concorde or arising in problems of physical acoustics, however, have significantly larger thickness so that continuum

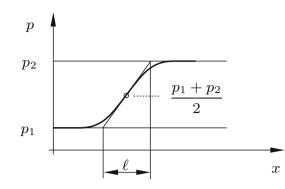


Fig. 15 Definition of shock thickness ℓ

Table 1 Estimates of shock thickness in air: $p_1 = 1$ bar, $T_1 = 0$ °C, $w_1 = 330$ m/s, $\gamma = 1.4$, $\lambda = 0.0024$ mkg/K, $c_p = 1005 \text{ m}^2 \text{s}^{-2} \text{K}^{-1}$, mean free path $\sim 6 \times 10^{-5}$ mm

$p_2 - p_1$ (bar)	ℓ (mm)	
$\sim 2 \times 10^{-1}$	$\sim 5 \times 10^{-5}$	Prandtl's "mittlere Verhältnisse"
$\sim 2 \times 10^{-3}$	$\sim 10^{-2}$	Sonic boom of Concorde
$\sim 2 \times 10^{-5}$	~ 1	Physical Acoustics

theory definitely applies. It is, therefore, of importance to investigate the effect of internal friction neglected by Prandtl.

This was achieved 4 years later in an independent study by Taylor [67]. The resulting structure equation

$$\delta \frac{dp}{dx} = (p - p_1)(p_2 - p), \quad \delta = \frac{\gamma - 1}{\gamma + 1} \frac{2w_1\lambda}{c_p} + \frac{2\rho_1w_1}{\gamma + 1} \frac{4\nu}{3}$$
(34)

is of exactly the same form as the one derived by Prandtl [50] with the only difference that the constant δ contains an additional term which involves the kinematic viscosity ν .

The structure equations derived by Prandtl and Taylor allow for an interesting observation. For $\delta = 0$ solutions are $p = p_1$ and $p = p_2$ which yields the pressure jump occurring in non-dissipative flows. Thus the structure equation is obtained simply by adding the dissipative term $\delta d p/dx$ to the equation which governs this type of flow. That this is true also for unsteady flows, i.e., acoustic waves of small, but finite amplitude which propagate into a state of rest characterized by the subscript 0 has been demonstrated by Lighthill [41]:

$$\frac{\partial p}{\partial t} + c_0 \left(1 + \frac{\gamma + 1}{2} \frac{p - p_0}{\rho_0 a_0^2} \right) \frac{\partial p}{\partial x} = \frac{\delta}{2} \frac{\partial^2 p}{\partial x^2}$$
(35)

Here the left hand side describes the formation and interaction shocks in inviscid and non-conducting perfect gases which are regularized by the term on the right-hand side already known from the pioneering investigations by Prandtl [50] and Taylor [67]. In my opinion this is a most remarkable result which still holds if we now turn to the case of general fluids including BZT fluids. As before the term on the left hand side of the structure equation, Cramer and Crickenberger [8], Kluwick [23]

$$\frac{\partial p}{\partial t} + \frac{\partial j(p)}{\partial x} = \frac{\delta}{2} \frac{\partial^2 p}{\partial x^2}, \quad j(p) = \frac{\Gamma_0}{2} p^2 + \frac{\Lambda_0}{6} p^3 + \frac{N_0}{24} p^4$$
(36)

governs the motion of jump discontinuities which propagate in non-dissipative media. The dynamics of such flows, however, is significantly more complex than before as it involves both classical and non-classical shocks, their mutual interaction and the phenomenon of shock splitting. All this complicated flow behavior can be captured if the quadratic nonlinearity which enters the theory of perfect gases is generalized, i.e., is replaced by a polynomial of fourth order. Herein Γ_0 , the fundamental derivative of gas dynamics, characterizes the curvature of isentropes in the p, v-diagram evaluated in the unperturbed state while Λ_0 and N_0 account for higher-order derivatives. In contrast, the right-hand side of the structure remains unchanged and still fulfills its task to regularize all these different types of jump discontinuities arising from the theory of non-dissipative

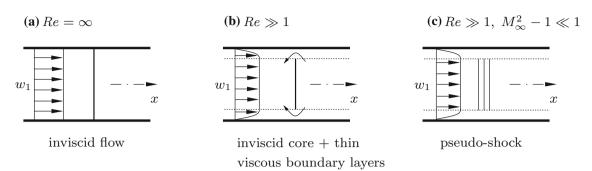


Fig. 16 Pseudo-shock in transonic slender channel flow

flows. A discussion of solutions of Eq. (36) is beyond the scope of this overview, but the most important conclusion relevant within this context is: The extended wave speed ordering relationship guarantees the existence of shock profiles in general fluids and, therefore, is sufficient to select jump discontinuities which are realizable physically.

The mechanism of shock regularization outlined so far applies to unconfined flows. In confined flows where wall effects can no longer be neglected a significantly different shock regularization mechanism comes into play. A representative example is provided by high Reynolds number flows in slender channels, Fig. 16. In the inviscid limit $Re = \infty$, a normal shock separates regions of supersonic and subsonic flow, Fig. 16a. For finite but large values of Re the flow exhibits a two-layer structure: an inviscid core and thin viscous wall layers required to satisfy the no slip at the wall, Fig. 16b. As a consequence the flow close to the wall is subsonic and pressure disturbances generated by the pressure jump across the shock in the inviscid core region will propagate upstream and thus modify the conditions of the incoming supersonic flow. For laminar flow this effect of upstream influence has been clarified first by Oswatitsch and Wieghardt [48] and is now known as Oswatitsch–Wieghardt mechanism, Lighthill [42]. In the case of transonic flow $M_1^2 - 1 \ll 1$ where wave fronts (characteristics) in the incoming unperturbed flow are almost perpendicular to the channel axis weak shocks are completely regularized, i.e., the shock discontinuity is replaced by a smooth pseudo-shock, Fig. 16c. The fluid motion inside the core region then is governed by the lossless version of the wave equation (36)

$$\frac{\partial p}{\partial t} + \frac{\partial j(p)}{\partial x} = \Lambda \frac{\partial A}{\partial x},\tag{37}$$

where the additional term on the right-hand side accounts for the reduction of the available area of cross section due to the presence of viscous wall layers and the similarity parameter $\Lambda = \Lambda(M_1, Re)$ measures the intensity of the resulting viscous-inviscid interaction. The wave equation (37) is embedded in a boundary layer problem which provides a second relationship between p and the perturbation displacement thickness -A and closes the flow description, Gittler and Kluwick [12], Kluwick and Gittler [26], Kluwick, Braun and Gittler [27], Kluwick and Meyer [32,33]. We thus conclude that the physical mechanism for the formation of pseudo-shocks reflects a subtle interplay of disturbances propagating upstream inside the wall layers which are slowly convected downstream in the core region where the flow is nearly sonic. Therefore, viscous shear stresses play a decisive role while viscous normal stresses, which are of prime importance in unconfined flows, are negligible small.

Results for pseudo-shocks of compressive and expansive type are displayed in Fig. 17. All quantities are suitably scaled and the overall pressure jump is normalized to ± 1 . In the case of compressive flow, the pressure rise, as expected, causes the perturbation displacement thickness – A to increase and the wall shear τ_w to decrease. Also the shock strength is large enough to generate a short separation bubble where τ_w is negative. In contrast the pressure reduction across the rarefaction pseudo-shock leads to a local maximum of the wall shear and boundary layer separation is not an issue as pointed out before in Sect. 6.

8 Conclusion and outlook

The puzzling problem concerning the existence of shock discontinuities has attracted many prominent scientists including Poisson [49] who triggered the discussion, Stokes [64] who considered a surface of discontinuity a natural supposition, Riemann [55] who demonstrated that shocks form naturally in compression waves,

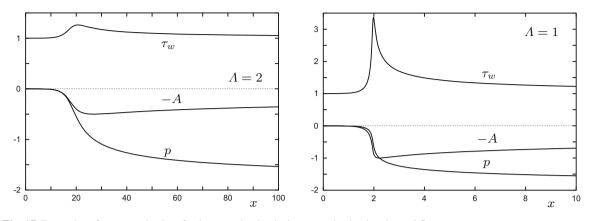


Fig. 17 Examples of compression/rarefaction pseudo-shocks in transonic slender channel flow

Rayleigh (1877) who objected based on arguments that such discontinuities violate conservation of energy, an argument followed by Lamb [36] as late as 1932 although this point of controversy had been clarified by Zemplén [76,77] as acknowledged by Rayleigh [65] and algebraic shock jump relationships had been derived already by Rankine [53] and Hugoniot [15,16]. Zemplén [76,77] also formulated the first modern definition of a shock wave:

"A shock wave is a surface of discontinuity propagating in a gas at which density and velocity experience abrupt changes. One can imagine two types of shock waves: (positive) compression shocks which propagate into the direction where the density of the gas is a minimum, and (negative) rarefaction waves which propagate into the direction of maximum density."

The role of isentropic curvature for shocks in arbitrary rather than perfect gases was considered first by Duhem [9] who focused on weak discontinuities, Becker [1] who clarified the process of shock formation and Bethe [3] who showed that van der Waals gases admit rarefaction shocks if the specific heat at constant volume is sufficiently large but considered the required values as unrealistic high and Thompson [68], Lambrakis and Thompson [37], Thompson and Lambrakis [70] who demonstrated the existence of real fluids where rarefaction shocks may form.

Stimulated by the experimental work of Stodola [63] the dissipative shock structure was calculated first for perfect gases by Prandtl [50] who took into account heat conduction only, Taylor [67] who also included the effect of viscous stresses, and for weak propagating shocks by Lighthill [41].

Real fluid effects on the structure of shock waves has been investigated first by Weyl [73] and in more detail by Gilbarg [13] who proved the existence and uniqueness of shock layer solutions for the class of fluids considered by Weyl [73] with the property that Γ is strictly positive. The shock layer problem for fluids with embedded negative Γ regions has been treated by Cramer and Crickenberger [8]. Lighthill's [41] work for shocks of small but finite amplitude was generalized by Cramer and Kluwick [7], Cramer and Crickenberger [8], while the structure of weak shocks in confined geometries was elucidated by Kluwick and Gittler [26], Kluwick, Braun and Gittler [27], Kluwick and Meyer [32,33].

The present review paper focuses on non-classical flow phenomena in the single-phase dense gas region of fluids with moderate and high molecular complexity. Related phenomena including mixed waves and rarefaction shocks, however, may occur also in the vapor–liquid critical region of pure liquids, e.g., Gulen, Thompson and Cho [14]. Their study is severely hampered by the fact that the usual analyticity requirements on which classical equations of state are based are not satisfied at the critical point. Specific equations of state for the critical region have been proposed by various authors. According to Widom [74] the full range of non-classical behavior can be accounted for if the free energy in the neighborhood of the critical point is written as a homogeneous function of its variables ρ , T. This suggestion is consistent with the hypothesis of scale invariance and can, as pointed out by Schoefield [60], be used to derive an especially useful parametric representation of the equation of state. By exploiting this result the properties of Γ in the single-phase region have been determined by Kluwick [22] as the leading order term of an asymptotic expansion holding in the limit as the critical point is approached. Significant further progress has been achieved by Nannan [44], Nannan et al. [45] who extended the analysis to cover the full vapor–liquid equilibrium region. Their findings provide a firm basis for the treatment of weakly nonlinear waves and the theoretical prediction of non-classical effects, Nannan et al. [46].

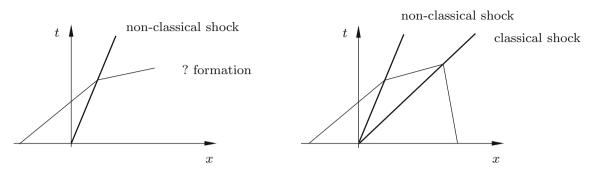


Fig. 18 Under-compressive non-classical shocks: single non-classical shock (left) violates, compound structure (right) satisfies wave speed ordering relationship

Applying a simple thought experiment, Kluwick [31] showed that the form of the structure equation for transonic internal flow carries over almost unchanged to high Reynolds number laminar flows of liquid films if the Froude number Fr differs only slightly from the critical value 1 (in the case of inviscid flow the similarity between compressible channel and incompressible free surface flow was recognized first by Joguet [20], Preiswerk [52] and Prandtl [51]). The right-hand side of the structure equation for weak hydraulic jumps, however, contains an additional dispersive term $W \partial^2 p / \partial x^2$, W = W(Fr, Re) which captures the effect of the finite pressure jump across the free surface due to surface tension, Kluwick [31], Kluwick, Exner, Cox and Grinschgl [30]. With increasing importance of surface tension, one observes the transition from monotonic to undular bores, but the speed ordering relationship (29), with M replaced by Fr, still provides a necessary condition to eliminate inadmissible jump discontinuities which may be predicted by the theory of inviscid, non-dispersive flows. This is no longer the case in general for liquid films which consist of two layers with different densities, Kluwick and Viertl [28], Kluwick, Scheichl and Cox [29], Kluwick, Szeywerth, Braun and Cox [34,35], Scheichl, Kluwick and Cox [59]. Then solutions of the structure equation exist which violate the speed ordering relationship so that waves pass through rather than converge toward surfaces of discontinuity which form if viscosity and surface tension are neglected, Fig. 18(a). Jump discontinuities characterized by this unconventional property are termed non-classical under-compressive shocks and have been predicted also for creeping flows, Bertozzi, Münch and Shearer [2], suspensions of particles in liquids, Kluwick, Cox and Scheichl [24], constrained two-layer flows, Segin, Tilley and Kondic [61], dense gas acoustics, Scheichl and Kluwick [57,58] and the continuum theory of pedestrian flow, Colombo and Rosini [5]. Readers interested in a more rigerous mathematical theory of under-compressive non-classical shocks are referred to the review papers by LeFloch [40] and El, Hoefer, Shearer [11] which also include applications from other fields such as nonlinear elasticity and nonlinear optics. Due to the existence of a continuous inner structure such discontinuities areaccording to the third criterion listed in Sect. 4—admissible. But then the question arises: how can such shocks form inside the fluid if the only known mechanism by intersecting wave fronts does not apply? A possible solution is that non-classical under-compressive shocks do not arise as single shocks but in combination with classical partners such that the resulting compound structure then indeed satisfies the speed ordering relationship, Fig. 18(b). For suspensions, this has been demonstrated by Cox and Kluwick [6], but if this new mechanism applies for other types of flows as well remains an open question. For hydraulic jumps in single-layer and two-layer flows, however, a first step has been taken more recently by Viertl [71], Kluwick, Szeywerth, Braun and Cox [34,35] who showed that in the limit of weak interaction and strong dispersion the perturbation displacement thickness due to the presence of the viscous wall layer can be calculated analytically and takes the form

$$A \sim \frac{\Gamma(2/3)}{3\text{Ai}'(0)} \int_{-\infty}^{x} \frac{\partial p/\partial\xi}{(x-\xi)^{1/3}} \,\mathrm{d}\xi = \frac{1}{3\text{Ai}'(0)} \frac{\partial^{1/3} p}{\partial x^{1/3}},\tag{38}$$

where the notion "fractional derivative" of order r, see, e.g., Sugimoto [66], has been introduced. The structure equation then reduces to a single novel evolution equation for the pressure disturbances:

$$\frac{\partial p}{\partial t} + \frac{\partial j(p)}{\partial x} = \frac{\Lambda}{3\operatorname{Ai}'(0)} \frac{\partial^{-2/3} p}{\partial x^{-2/3}} + W \frac{\partial^3 p}{\partial x^3}.$$
(39)

Current research focuses on numerical solutions of Eq. (39) with special emphasis on the process of shock formation.

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