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Chapman–Jouguet hypothesis 1899–1999: One century between myth and reality

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Abstract. The 20$^{\text{th}}$ century saw the rapid development of quantum mechanics and micro-scales physics. However, classical mechanics did not lose any interest, and did not cease setting severe enigmas. Among them lies detonation, observed and measured since Berthelot (1881), but whose modeling required nearly hundred years of effort. Following the fashion of celebrations, we could say that the publication by Chapman in 1899 is a reason for rewriting, in modern terms, the main facts of past century: enhancing the few brilliant steps and also mentioning their sluggish diffusion, which arises from linguistic and national fractures within the scientific world and also reflects scientists' great reluctancy to recognize and overcome the intrinsic uncertainties of modeling.

Key words: Detonation, Chapman–Jouguet, Wave modeling

1 Wave modeling of reactive propagations

Considering, with hindsight, the phenomena of deflagration and detonation, and bearing in mind the modern ideas about state laws and constitutive equations and dissipative effects, we may undoubtedly say that Jouguet (1917) and his contemporaries had expressed, in their own clear words, the main features of wave modeling of chemically reactive flows.

1. A flow with detonation or deflagration may be ascribed the perfect fluid approximation, except for a narrow zone, moving through the system.
2. In the lap of this zone, the behaviour of the substance may still be ascribed the fluid – but non-perfect – approximation: dissipation effects are not negligeable therein, because of the deviation from chemical equilibrium and because of velocity and/or temperature gradients.
3. However, in the lap of this zone, the temperature rises so high and the changes in velocity, pressure, volume, etc., come out in the course of such a short path (ε fraction of the total observable path), that it is acceptable, in the frame of a global description, to consider this zone as an approximately geometrical surface discontinuity named a *wave*, upstream of which the flow is inert, and dowstream of which the flow is reactive under the permanent condition of chemical equilibrium.
4. In the frame of such modeling, the *local* theory of Hugoniot [2] is valid: *at any point of Σ at any time*
   – the jumps in pressure p, specific volume v, and specific internal energy e are linked by the Hugoniot relation

$$e - e_0 = \frac{1}{2}(p + p_0)(v_0 - v)\,, \tag{1}$$

   – the normal relative velocities w_0 (upstream) and w (downstream) are given by

$$w_0 = v_0\sqrt{(p - p_0)/(v_0 - v)}\,, \tag{2a}$$

$$w = v\sqrt{(p - p_0)/(v_0 - v)}\,, \tag{2b}$$

   where the normal to Σ is oriented from upstream towards downstream.

2 Crussard curve and critical waves

After emphasizing how advanced the description synthesized by Jouguet in his *Mécanique des explosifs* (1917) is, it is proper to put the remainder in its proper light, since there lie the origins of misunderstandings that will hang heavily on the development of ideas.

For one reason at least (i.e. the available observations at the turn of the century dealt with only gaseous systems considered under normal conditions of pressure and temperature), Jouguet did not move away from the assumption under which the detonation products behave with a constant γ ideal gas equation of state, $e = pv/(\gamma - 1)$, whose representation in (v, p, e) space is hyperboloid (D). As a consequence, he faced a very simple analytical situation:

(i) Crussard curve (H), drawn over (D) as a result of (1), is 'fair' enough to be projected on the (v, p) plane as a hyperbola (H'),

(ii) given an upstream state (v_0, p_0) and an upstream relative normal velocity w_0, determination of possible downstream states results from a familiar discussion: intersection of hyperbola (H') with a line originating from (v_0, p_0) with slope $-\rho_0 w_0^2$.

Despite its obvious over-simplification, this discussion has the indisputable merit of dividing, for the first time, the substances in two categories according to whether it is possible or not to draw two tangent lines to (H') from point $A(v_0, p_0)$ (for reasons which appear only at some advanced status of theory, this division is no less than that between explosive and non-explosive substances). In the first case, the contact points on (H') of the tangent lines determine waves named 'critical' by Crussard (1907), with which correspond two downstream states on curve (H) itself. These states were named, much later, 'Chapman–Jouguet' states. For the sake of simplicity, we shall call J the one related to a detonation $(p > p_0)$; the value of w_0 at J will be written D_*. More generally, any quantity at J will be marked with subscript $_*$.

On top of this beautiful geometrical definition of point J, come other remarkable physical features.

– One is mentioned by Chapman (1899): J is the point on (H) where the upstream relative normal velocity w_0 is minimum.
– Another is given by Crussard (1907): J is the point on (H) where the downstream relative normal velocity w is equal to the local downstream sound velocity a.
– The last is demonstrated by Jouguet (1917): at any point on (H) where $p > p_*$ $(p < p_*)$, the ratio w/a is less (more) than unity.

So many wonderful attributes would not have been sufficiant for J to become, for decades, the cornerstone of all detonation theories if the experimental results in tubes, which Jouguet was aware of, had not strengthened its singularity and suggested the 'hypothesis': J does represent the downstream state to be assigned to the detonation products of an *explosive wave* (Jouguet, p. 326) defined as a propagation (i) *indifferent to limiting rear conditions* (ii) *in the form of a constant velocity translation.* On pages 332 and 333 of Jouguet's work, tables I and II set forth twenty gaseous mixtures where the measured velocity agrees within experimental error with the computed velocity D_*.

But several pages, 300 to 316, where Jouguet discusses the "possibility of shock and combustion waves" show indisputedly that he never thought of his 'hypothesis' as a 'law' whose validity would extend to all propagation regimes.

3 Birth of a myth

There occur the first tricks of history, ... and failings of men, were they scientists. Let us pick up some lines of the introduction in *Detonation of condensed explosives* (Chéret, 1993).

"After smouldering under the embers of the first World War, research was revived outside France as witnessed by the works, which have become classics, of N.N. Semenov (1928), B. Lewis and G. Von Elbe (1938), and W. Jost (1939). All three, in contrast to the view of E. Jouguet, which is synthetic and thermodynamic in nature, apply themselves to a review of known phenomena and their kinetic aspects.
From 1940, the needs of nations involved in the Second World War created a rapid and unprecedented expansion in research into solid explosives. The use of such explosives in nuclear weapons necessitated the characterization of their properties and a modeling of their effects, which in turn meant resorting to the most highly developed methods of physics... and to the most brilliant minds of the time. The papers of Y.B. Zeldovitch (1940), G.I. Taylor (1941), J. Von Neumann (1942), and W. Döring (1943) date from these troubled years. Although the papers were written in an isolation which we may only guess at, they share a common characteristic – they abandon the kinetic aspect envisaged during the interwar years and return to the only existing theory, that of E. Jouguet, to try to prove its obscure points or to draw from it simple conclusions".

But unfortunately, the authors have another common feature, that is, not being able or willing (lack of time? lack of French original text or of faithful translation) to deepen Jouguet's arguments. In the following decades, the memoirs still enhance the deficiency: thus the idea of Chapman–Jouguet 'law' flourishes as a belief that the work by the first as well as by the second guarantees some well-established law, according to which one and the same detonation velocity exists: D_*.

Yet, experimental results – especially dealing with TNT and RDX based compositions – had been stored in the 1940s and should have led to such over-simplification being dispelled. Were they not saying that a translation velocity $\delta\vec{i}$ is observed in a tube with axis $\vec{i}$, that δ changes when the diameter is varied, and does not accomodate with a 'law' endowed with a unique value of velocity? Were they not saying also that the wave in a tube is an $\vec{i}$-axisymmetric surface, whose concavity faces the detonation products, from which follows that a translation-type propagation where $\delta = D_*$, would mean that the normal relative velocity $w_0 = \delta \cos \Psi$ equals D_* on the axis $(\Psi = 0)$, but inexorably deviates from D_* outside the axis $(\Psi > 0)$ and then takes values smaller than D_*, which are incompatible with admissible downstream states on (H_+)?

Actually, such a gap between experimental results and the Chapman–Jouguet 'law' is not unknown even by the most enthusiastic users, and does not leave them unconcerned. But, surprisingly enough, none of them goes back to the origins; all of them have chosen an escape way and state that, instead of being 'completely' true, the Chapman–Jouguet 'law' is 'asymptotically' true, i.e. when the flow is plane and steady. Such a statement, apart from being pure conjecture, means a dramatic twofold regression: (a) first as regards the ambition shown by the authors early in the century, who, following the spirit of Hugoniot's *local* analysis, aimed at finding some downstream state at each point of the wave, whatever the spatial and time features of the *overall flow* were; (b) also as regards the general development of theorical physics and the blossoming of scaling laws. As a matter of fact, in 1949, Hermann Weyl gives a wide diffusion to ideas expressed as early as 1944, on the right way of setting the equations of internal structure of a shock layer through an appropriate $1/\varepsilon$ stretching along the normal line to Σ. As early as 1946, K.O. Friedrichs alone, and then in 1948 R. Courant and K.O. Friedrichs together, extend the ideas of Weyl to detonations, and show that the actual existence of an internal structure ending at a downstream state of (H) is a prerequisite of wave modeling of propagation. Their dissertation means that, *a contrario*, putting up with no actual marking of a downstream state on (H) deprives the model of any operative significance.

By way of an anecdote, let us mention two other escape-routes, which are put forward in order to dodge the difficulties linked with the Chapman–Jouguet 'law'. One consists in incriminating the explosive substance itself, and in making a difference between ideal explosives (which are 'good' enough and respectful of the 'law') and non-ideal explosives; these labels are still in use! Another one consists in incriminating the chemical equilibrium assumption, and in maintaining that, in any circumstance, the downstream state is endowed with a downstream relative normal velocity w identical to some local 'frozen' sound velocity a ('frozen' means that a is computed without acknowledging the chemical equilibrium equations, i.e. without making use of the correlation between chemical concentrations and state variables!); such an alteration, in addition to the fact that it despises a great number of experimental results, destroys the consistency of the model since it tolerates, beyond the 'downstream state', some finite chemical dissipation effect!

4 Inexorable uncertainties

Such passion for establishing the Chapman–Jouguet 'law' and keeping it at the expense of intellectual contortions deserves an explanation mostly grounded on human laziness, summarized below in the form of three questions:

– Why should we deny ourselves a law that is indeed imperfect since it is inconsistent with some experimental results, but that brings somewhat satisfactory predictive results for a great many applications?
– Why should we not hope for a simple detonation theory like Bethe's shock theory (1942) which shows that, given an upstream state, there exists one and only one downstream state whenever it is assigned to ensure coincidence between the value of the relative normal upstream velocity and the measured value.
– Why should we not hope, as a consequence of above wish, to escape two difficult problems:
  (i) make a choice between those two downstream states, which ensure coincidence between the value of the relative normal upstream and a measured value higher than D_*;
  (ii) make a guess for the absence of a downstream state when the measured velocity is lower than D_*.

Actually this laziness keeps close to basic theoretical difficulties.

The wave modeling of detonation essentially ignores the details of the internal structure that leads from the upstream state to the downstream state, but does not preclude that the downstream state itself results from the *matching* between this internal structure and the remainder of the flow-including boundary conditions. This is exactly the kind of argument which is given by K.O. Friedrichs (1946) when he denies the states $(H_+, p < p_*)$ any physical meaning and thus answers question (i).

The wave modeling of detonation surrenders any pretention to determining the downstream state (p, v, e) and the corresponding relative normal velocities w and w_0 better than within $O(\varepsilon)$; in other words, modeling does not preclude that the downstream state, while matching some external flow, leads through (2.a) to a normal relative upstream velocity w_0, which may deviate within $O(\varepsilon)$ from the measured velocity D, at any point P of wave surface Σ. In other words again, the measured velocity $D(P)$ is not necessarily the one to be substituted for w_0 in (2.a) when looking for the downstream state. This last remark is, obviously, an answer to question (ii).

5 Strong and quasi C–J detonations

The above considerations show that wave modeling of a detonation is compatible with two and only two cases:

– either w_0 is assigned a value higher than D_*; then the downstream state belongs to $(H_+, p > p_*)$ and consequently the thus modeled detonation deserves the epithet *strong*;
– or w_0 is assigned the value D_*; then the downstream state is a C–J state, but $D(P) = D_*[1 + O(\varepsilon)]$, which implies to give the name *quasi C–J* to thus modeled detonation.

The $O(\varepsilon)$ quantity appears to 'measure' the *normalized effect* of dissipative phenomena on the relative upstream normal velocity. Thus, other things being equal, it 'measures' the geometrical effect (sphericity effect for spherical detonation, diameter effect for tube or rod detonation, etc.). Thus, for given dimensions, it measures the mesostructural effects (grain distribution, void distribution, crystallite facies, relative orientation of propagation and crystal, etc.). *A contrario*, given the macroscopic features of an explosive system, the wave modeling will be the same for two propagations different from one another only through mesostructural features, either from the very origin of the system, or later on due to aging. We shall investigate this statement and its consequences in the epilogue.

It is easily understood that the quantity $O(\varepsilon)$, the normalized summation of varied dissipative effects, is presently scarcely predicted and that even its sign remains unknown. In such a way that measuring $D(P)$ and comparing to D_* do not allow us to decide whether a detonation is *locally strong or quasi C–J*. The decision is to be taken only as a result of a deep analysis of the *whole flow*, when using scaling laws and having recourse to the matched asymptotic expansions (MAE) method.

6 Matched asymptotic expansions and propagation rule

The MAE method has given birth and unity to a wide field, which includes especially the boundary layer, shock layer and detonation layer. We are not going to visit the founding texts, nor the developments in Chéret (1971, 1993), dealing specifically with detonation. We just recall that, when addressing the question 'given a detonation, is it to be considered strong or quasi-C–J?', the MAE method provides us with a local answer: 'at point $P \in \Sigma$ with positive mean curvature, an autonomous detonation is quasi-C–J; at point $P \in \Sigma$ with negative mean curvature, detonation is strong'.

This rule, *which must be regarded as a theorem*, is better understood and applied when complemented with the definitions below.

(a) The mean curvature is algebraic and equal to

$$\frac{1}{2}\left[\frac{1}{\vec{PC_1},\,\vec{N}}+\frac{1}{\vec{PC_2},\,\vec{N}}\right],$$

where $\vec{N}$ stands for the normal at P to Σ and is directed from upstream to downstream, where C_1 and C_2 stand for the two main curvature centers of Σ at P.

(b) A detonation is *autonomous* when the field of normal velocities is decelerated in the near downstream flow. N.B. Refering to the usual conditions on priming boundaries and free boundaries of usual explosive devices, experiment shows the autonomous nature of detonation. However, should some overmighty spherical constantly expanding priming device be available, non-autonomous spherically diverging detonation may occur (Chéret, 1993, p. 83).

A few examples, drawn from usual experimental work, allow us to illustrate and demonstrate the pertinency of the rule.

– Spherically converging detonation exhibits uniform negative mean curvature, consequently it is strong (Chéret, 1993, p. 88).
– Spherically diverging detonation exhibits uniform positive mean curvature. Whenever the central boundary velocity is less than some critical value, then it is autonomous and consequently quasi-C–J. Whenever the central boundary velocity is higher than that critical value, then it is strong (Chéret, 1993, p. 83). What a nice example of bifurcation!
– End priming of a rod turns into an autonomous detonation whose mean curvature is positive everywhere, consequently it is uniformly quasi-C–J (Chéret, 1993, p. 308).
– Lateral priming of a rod turns into an autonomous detonation whose mean curvature – whenever lateral velocity is properly chosen – is negative in the vicinity of the axis and positive elsewhere, consequently it is strong near the axis and quasi-C–J elsewhere (Chéret, 1993, p. 311).

These four examples bear evidence that the strong or quasi-C–J nature is a local feature of the detonation, and that conditions on the boundaries of the flow may be of determinant or even critical importance.

7 Epilogue

One hundred years after Chapman's letter, is it possible to say that reality has triumphed over myth? Alas, no, since models are still developed that strive to patch up the Chapman-Jouguet 'law'.

No doubt that *errare humanum est* and that the scientist who explores dead-end paths before finding the way through does not escape the common human condition; no doubt either that *persevarere diabolicum*.

This persistancy in error is all the more heart-breaking because of the long-lasting evidence of wave-modeling of detonation being unable to provide for a detailed prediction of the actual propagation $D(P,t)$ and of the influence of mesostructural parameters on the propagation. This inability is yet implicitly known since those numerical simulations which are based on front tracking do not succeed in matching computed progression and observed progression, unless they throw away unicity and universality of the equation of state of the detonation products!

Does this mean that there is no other salvation than 3-D dissipative codes? In my opinion, no, on the contrary. I am convinced that such codes will reach predictive ability well after physicists have got insight into $O(\varepsilon)$ within the frame of simple configurations, an example of which is given in *Detonation of condensed explosives* (Chéret, 1993, p. 98). One should not need one century more if one uses the phenomena which underlie the internal structure: the so-called ZND ignitor shock, and appropriate reactivity (Chéret, 1993, p. 204).

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