## CJ AND ZND MODELS: MODELS AGAINST BASIC THERMODYNAMIC PRINCIPLES

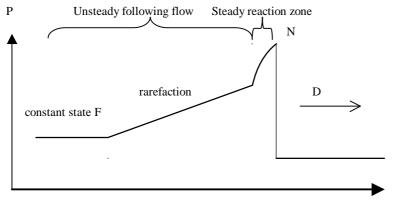
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## EXTENDED ABSTRACT

Thermodynamics is a fundamental part of all physical science. CJ and ZND models violate the basic principles of thermodynamics.

Following is a typical configuration of the detonation wave described in the CJ and ZND models [1],[2].



Distance X

1.1. According to CJ and ZND models, entropy has the minimum at the end of detonation process.

According to CJ and ZND models, the entropy at the CJ point is the minimum in Hugoniot curve. In the whole unsteady following flow, the main part of the system after detonation wave sweeps over, the entropy is constant throughout at the CJ value. The Hugoniot curve is the locus of all possible final states for any detonation [1],[2]. Therefore, according to CJ and ZND

models, the entropy of final explosion products is the minimum among all of possible states after front. The entropy of detonation process, a typical spontaneous process, goes towards the minimum as described in CJ and ZND models.

Minimum entropy implies minimum disorder, i.e., agitated by the most violent perturbation in the reaction zone, the final explosion products are in the lowest disordered state.

Minimum entropy means minimum probability, i.e., the detonation process proceeds towards an end of the minimum probability among all of possible ones. It is well known that an event with minimum probability implies a nearly impossible event in stochastic theory.

Minimum entropy means minimum irreversibility. Being a typical thermal spontaneous phenomenon with the greatest and the fastest heat release, the detonation process, to one's surprise, is a process with the minimum irreversibility!

1.2. According to CJ and ZND models, system does not tend to equilibrium state and will never reach it.

The tendency towards equilibrium is so important to physics that the second law is probably the most universal regulator of natural activities known to science [3].

It is certain that the unsteady following flow is not in the equilibrium state, for there are pressure, temperature, density distributions, and particles of explosive products move forward orderly in one direction. Unfortunately, according to the CJ and ZND models, although it is not in the equilibrium state, the unsteady following flow has all of the equilibrium features:

$$S = \max$$
$$\frac{dS}{dt} = 0$$
$$\frac{d^2S}{dt^2} \le 0$$

According to thermodynamics, an irreversible process taking place

inside a system always lower the value of entropy production per unit time [4]. Since the entropy production in the whole unsteady following flow is already down to zero, it will not rise again, i.e., the system cannot develop further and will never reach the equilibrium state.

1.3. According to CJ and ZND models, entropy increase rate is the slowest one.

Entropy has the minimum at CJ point, therefore entropy increases most slowly while the process goes to CJ point.

Spontaneous process shall go in the direction that makes entropy increase fastest, i.e., go to the direction of gradient of potential [4]:

$$\frac{d_i S}{dt} = \sum_k J_k X_k > 0$$

here the "force"  $X_k$  is the gradient of thermodynamic potentials.

Faced with many possible paths, the CJ and ZND models prefer to choose the one with the slowest rate of entropy increase, rather than the one with the fastest rate.

1.4. CJ and ZND models prove a nearly impossible state is stable.

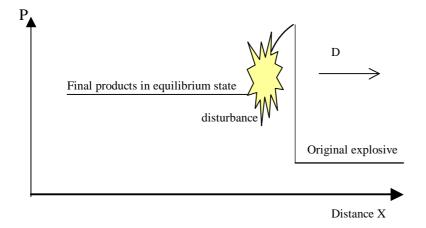
A little disturbance divergent from CJ point will make entropy increase, i.e., for any D>D<sub>CJ</sub> we always have dS > 0. According to Gibbs-Duhem stability criterion[5], CJ state is certainly an unstable one.

CJ state has the minimum entropy, i.e., it exists with the minimum probability, however, CJ and ZND models go so far as to prove this nearly impossible state is stable using the "rarefaction" theorem.

2. It is necessary to recognize the entropy law to be the premier one in science.

All of the words mentioned above about thermodynamics are commonplace knowledge well known by students. The property that entropy at the CJ point is the minimum in Hugoniot curve is also mentioned by all of the monographs concerning detonation. Unfortunately, no attention has been paid to these absurdities. In CJ and ZND models, it is assumed that the flow is one-dimensional, i.e., the particles of explosion products are assumed to move only in one direction: towards the front. Moving in one direction means in good order, means queuing up forward. Under this assumption, minimum entropy is doomed at the end. It is this assumption that creates these absurdities.

The detonation wave is one of the most violent perturbations in nature. Any system that is subjected to random agitations will eventually attain its most disordered state, i.e., shall go towards equilibrium state. It is necessary to construct a new detonation model complying with basic thermodynamics principles. Detonation models shall reflect the essence of detonation wave: particles of explosive products in reaction zone shall move disorderly and the system shall go towards equilibrium.



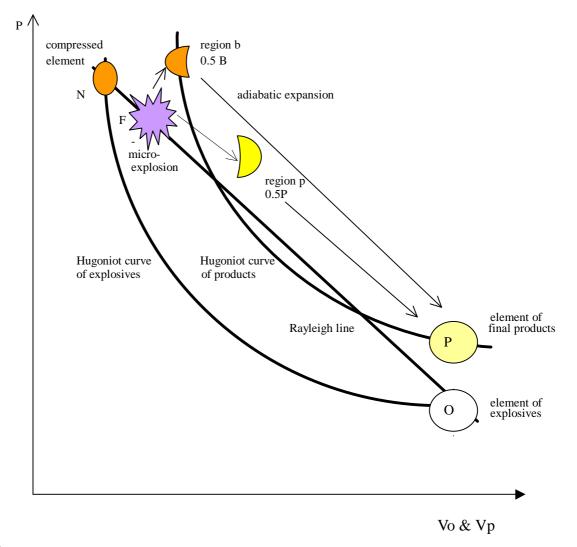
According to these principles, many models can be proposed to describe how released chemical energy creates disorder, i.e., a large number of detonation models will be established. Among these models, conjugate detonation model proposed by the author [6](See above Fig.), may not be the best one, but is the first one that recognizes thermodynamic equilibrium state is the end state of detonation process. Conjugate model considers detonation process goes in following steps:

 $O \rightarrow N \rightarrow F$ , compression, expansion and reaction, that are exactly the same as in CJ and ZND models;

 $F \rightarrow (0.5B+0.5P)$ , micro-explosion takes place, which makes the

explosive element be divided into two regions called conjugate pairs in different temperature, pressure, density, and move in different velocities.

 $(0.5B+0.5P) \rightarrow P$ , region b expanses and the conjugate pairs annihilate.



## References

[1] W.C. Davis	Sci. Am.,	1987, 256(5): 106-112

[2] W. Fickett & W.C. Davis DETONATION 1979

[3] The New Encyclopedia Britannica. 15<sup>th</sup> Edition. 1985

[4] I. Prigogine. Introduction to thermodynamics of irreversible Process 1967.[5] P.Glansdorff, I. Prigogine.

Thermodynamic theory of structure, stability, and fluctuations.1971

[6]Hu,Shaoming. Proceedings of the 28th International Pyrotechnics Seminar. 2001. 353-364