

**COMMITTEE I**

Unity of Science: Organization and  
Change in Complex Systems

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**BENARD CONVECTION, TURBULENCE AND  
CHEMICAL REACTIONS**

by

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**DISCUSSION PAPER**

on

Manuel G. Velarde's  
Self Organization and Evolution through Fluctuations and Instabilities

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Professor Velarde's contribution covers broadly a variety of topics concerned with biological and inanimate matter evolution and definitions of terms used to describe transitions to far from equilibrium states. His central contribution is a brief description of Benard convection and turbulence. Finally, he offers some reflections on the relationship of chaotic evolution with Economics and Sociology.

My task is that of reviewing the essentials of these two phenomena with the purpose of emphasizing certain thermodynamic aspects.

I agree with Professor Velarde's statements in his introduction when he emphasizes the fact that the great progresses achieved in the fields of statistical mechanics, non-equilibrium thermodynamics and the theoretical and experimental studies of non-equilibrium cooperative synergetic phenomena have led to new unifying concepts and models to clarify certain problems of self-organization and evolution through fluctuations and instabilities.

The instabilities in ~~steady~~ states are fine illustrations of processes of spontaneous self-organization. Reference is made to the Benard Instability which is originated by the vertical temperature gradient which is set up through a horizontal liquid layer heated from the bottom. The boundary conditions developed in the system because of the difference in temperature between the bottom and top of the layer originates an energy flux which moves from the bottom to the top. As soon as the gradient reaches a threshold value defined by the distance from equilibrium, the stationary state in which energy is conveyed by conduction alone, without any convection, becomes unstable, thus the system evolves to steady cellular convection of ensembles of molecules, thus increasing the rate of energy transfer. This new state constitutes a dissipative structure, to the extent that it is maintained as long as the energy flux is steady.

The existence of the temperature gradient is not sufficient to ensure the onset of convection flow. For convection to take place, the buoyancy <sup>which is due to gravity</sup> originated by this gradient must exceed the dissipative effects of viscous drag and heat diffusion. This transition takes place when the Rayleigh number exceeds a certain critical value.

This number is a dimensionless ratio of the buoyant force divided by the product of the viscous drag and the rate of heat diffusion.

The Benard convection is due undoubtedly to a phase transition far from thermodynamic equilibrium. The convection motion consists of a complex spatial organization of the system with an increase in entropy production. Exceedingly large numbers of molecules move coherently forming hexagonal convection cells of characteristic size.

One should notice that in the linear region, a system tends towards a steady state characterized by minimum entropy production. But in this case of a system far from equilibrium in which the fluxes are no longer linear functions of the forces, the system evolves towards a steady state which cannot be characterized in terms of the entropy production which is proper of near-equilibrium states.

The transition from disorder to order, that is, from a state of high entropy content towards one of low entropy content does not contradict the Second Law because the incoming energy  $U_1$  is accompanied by the low entropy  $S_1$  whereas the outgoing energy  $U_2$  which is usually equal to  $U_1$ , is accompanied by a very high entropy  $S_2$ . The important conclusion is that the total entropy of the <sup>open</sup> system and the energy flow can increase due to the increased entropy contained in the energy while at the same time, the entropy of the system can decrease due to the spontaneous creation of order within the system. This appears to be a characteristic of dissipative processes.

One aspect that appears to be interesting is the effect of the gravitational field on the transition from the chaotic structure towards the dissipative structures (the Benard cells). The instability of a Benard cell is the raising of the center of gravity as the result of thermal dilation. Thus, it is clear that gravitation plays an important function which leads to a new structure in spite of the fact that the Benard cells have a thickness of only a few millimeters. The effect of the gravitational force is negligible at equilibrium, but the far from equilibrium situation created by the gradient of temperature induces macroscopic effects which are discernible in the thin

liquid layer. Thus, it is evident that the far from equilibrium situation magnifies the effect of gravitation on the Benard phenomenon.

The other case cited by Professor Velarde of a system driven away far from equilibrium is turbulence, which was identified before as a case of disorder. Nowadays it is known as being due to a chaotic situation on the macroscopic scale, but highly organized on the microscopic scale. If the multiple space and time scales involved in turbulence correspond to a coherent behaviour of many millions of molecules, it does not make sense to speak of a deterministic chaos, but rather of deterministic consequences of the complexities of the phenomena involved.

One should recognize that the transition of laminar flow to turbulent flow is a process of self-organization. In this transition, part of the energy of the system which is included in the thermal motion of the molecules while they flow laminarily is transferred to macroscopic organized <sup>collective</sup> motion.

It is interesting to realize that the resistance which solid objects encounter when they are dragged or driven through any fluid (liquid or gas) at discernible velocity is proportional not to the first power but approximately to the square of the velocity. Thus, the law of viscous friction which is valid at low velocities with laminar flow does not at all apply to turbulent flow.

Osborne Reynolds discovered that the change from the first power law which is characteristic of laminar flow to the second power law which is characteristic of turbulent flow is not gradual but astonishingly sudden. He also found that this transition takes place in any fluid and for any given apparatus always at the same critical velocity. This transition from laminar to turbulent flow takes place at a sufficiently large distance from equilibrium. The threshold is measured by a certain value of the dimensionless Reynolds number ( $R = 2 \rho V / \pi \eta r t$ ).

I find it interesting to recognize the philosophical questions raised by Professor Velarde. He mentions that although the laws of a system may be purely deterministic, there is no possibility of predictability in the sense of Newton's paradigm. Then, he states that this lack of predictability of the future of the system is well-known by our meteorologists. This is confusing, for when a system is subject to deterministic laws it means that there is an invariant relationship between cause and effect in the primitive sense and in more advanced thought a timeless relation among variables applicable at any time with equal validity. The poor meteorologist cannot predict the climate of tomorrow with the greatest certainty for he does not yet know sufficiently about the variables that define weather.

Concerning chemical reactions a few reflexions are in order. It is known that a chemical reaction to an open system is subject to both external and internal variables. The external variables such as temperature and pressure determine the frequency of collision of the molecules in order for them to react through breaking and forming chemical bonds to originate intermediate structures and a final chemical compound. The internal parameter cannot operate independently of the external variables to determine the configurational behavior of the reacting system, thus recorded by the appropriate entropy variation.

A chemical reaction leads to entropy production contrary to the deterministic view and method of stating that if we know the initial concentrations, one should know at anytime how this parameter changes. This is particularly useful insofar as the system is at, or close to equilibrium. But when the reacting system is far from equilibrium, the deterministic description breaks down.

The conversion from a system in equilibrium or close to it to a far from equilibrium state takes place when the system surpasses a bifurcation point whereby the system is subject to a stochastic process. How the molecules decide to follow one path or the other is not known. What determines the path for them to follow remains to be established? for I believe that everything in existence is subject to nomological behavior. It appears to be a very significant contribution Prigogine's discovery that randomness is a condition to ordering.

We would want to know what is the relationship between the macroscopic levels and microscopic configurations insofar as they define a dissipative structure. How do the fluctuations operate to determine the final outcome of a chemical reaction?

To talk about reaction probabilities is proper in the sense of how the reactants act to give this or that compound, depending upon the external and internal variables, including the catalyst. To suggest, as Prigogine does, that one should build a statistical theory involving a distribution of reaction probabilities is a challenging proposition, once, it is not known yet what exactly determines the selectivity of a catalyst. To date, it is not even known what is the relationship between selectivity and reactivity of a catalyst.

The postnewtonian paradigm formulated by Prigogine of a world of atoms and molecules operating in an open system characterized by the free exchange of matter and energy where change and disorder are the determining factors ~~and that~~ <sup>of</sup> order, stability and equilibrium *which* ~~might be~~ <sup>are</sup> the outcome of a critical conversion signaled by bifurcation points is the medular material of a new epistemology.

To this moment, there is no hope that we shall know which is the finality of a system--for it might be that in a state of far from equilibrium, it might disintegrate, continue its path towards a new bifurcation point, or it might instead progress to a higher level of order. And all these, it is said that proceed spontaneously from disorder and chaos to highly ordered structures through a process of self-organization.

It would appear that we are back to Democrito as far as we accept the doctrine of change, to Aristotles as long as we adhere to a fundamental teleology, and to a doctrine of organismic analogies when it is suggested that the behavior of human society is an analogue of the behavior of atoms and molecules. Thus, so is the brave new world of science and philosophy!

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