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Causality principle, non-equilibrium thermodynamics and non-linear science of open systems

R P Rastogi* and R C Srivastava
Chemistry Department, Gorakhpur University, Gorakhpur 273 009

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In real life situations, open systems in non-equilibrium are sometimes in steady state and sometimes in non-steady states. Steady state is obtained when forces and counter forces interact. However, when multiple forces are operative involving autocatalysis (positive feedback) and inhibitory step (negative feedback), exotic non-equilibrium phenomena are observed. Extensive theoretical studies based on non-equilibrium thermodynamics and non-linear dynamics and experimental studies related to simple and complex non-equilibrium physico-chemical systems, which have possible application in real systems in nature, has been reported. Present paper intends to: i) Elucidate concepts related to causality principle developed on the basis of experimental and theoretical studies; and ii) To illustrate manner, in which multiple forces interact in phenomena involving multiple processes and multiple cause-effect sequence such as: a) non-equilibrium steady states; b) bifurcation from steady state to bi-stability and oscillatory state; c) temporal and spatio-temporal oscillations; d) chaos; and e) pattern formation and fractal growth in space.

Keywords: Causality principle, Non-equilibrium thermodynamics, Non-linear science, Open systems

Introduction

Living systems (social, political and economic including management, administration and governance) are never at equilibrium and can undergo changes due to small perturbations involving bifurcation from one state to another or states involving periodic variation in time and space. In this regard, issue has been raised whether science deals with real world[1]. Concept of social evolution is moving towards an interdisciplinary theory of change of state[2]. When system is disturbed, there is a tendency for self-organization[3]. Comprehensive studies have been reported[4] for analogous physico-chemical systems in non-equilibrium involving exotic transitions in complex systems such as: i) Steady state; ii) Switching to another steady state; iii) Variation of state with time with simple and complex periodicity; iv) Chaotic changes both deterministic and noisy; and v) Variation in the nature of state with respect to time and position. Physical basis of complexity in living, physiological, geological, social and economic systems involve following features: 1) Complex network of subsystems (continuous as well as discontinuous); 2) Multiple processes; 3) Multiple cause-effect relations (complex causal network); 4) Non-linear processes involving non-linear dynamics; 5) Frequent bifurcation from one state to another; 6) Complex time-dependence of time-variant state of typical systems; and 7) Complex time- and space order.

Non-equilibrium thermodynamics provides framework for development of theories, similar to derivation theories of causation[3,5,6]. Present paper analyzes data available in non-equilibrium science from regions close as well as very far from equilibrium. Primary objective is to examine causal relations in multiple cause-effect sequence to understand: i) Precise nature of cause and effect in simple and complex non-equilibrium systems; ii) Causal relation and nature of correlation coefficients (CC) between single cause and single effect; iii) Causal relations and nature of CCs when coupling between causes and effects takes place; iv) Variables, which influence magnitude of phenomenological coefficients (PCs); v) Role of cause and effect in typical non-equilibrium steady states within linear range; vi) Non-linear relationship between cause and effect in steady states beyond linear range; vii) Interdependence in multiple cause-effect systems; viii) Cause-effect network

*Author for correspondence
E-mail: rprastogi@yahoo.com

in complex non-equilibrium systems exhibiting bi-stability, time- and space-order; ix) Causal factors in chaos, noise and turbulence; and x) Complex growth phenomena in terms of causality principle.

Causality Principle in Epistemology

Causality simply means that effect follows the cause. Thus, cause must be prior to, or at least simultaneous with the effect. According to Popper[7a] "The principle of causality is assertion that any event whatsoever can be causally explained, that is it can be deductively predicted". Philosophically, concept of causality has been a complex one. According to Aristotle[7b], major causes may be classified as follows: i) Material cause; ii) Formal cause; iii) Efficient cause; and iv) Final cause. This communication is concerned with efficient cause, which covers agent, particular causal event or relevant causal state of affairs.

Theology puts material cause to be God. Early Indian thinkers[8a] had been mainly concerned with material cause in the context of evolution and origin of universe[6]. Diametrically, opposite views have been proposed as: i) According to 'Satkaryavad', effect is already existent in the cause (Sankhya and Vedanta system of philosophy support it); and ii) According to 'Asatkaryavad', effect is absolutely non-existent in the cause (Nyaya and Budha system of philosophy support it). According to Sankhya system[8b], "that which invariably precedes an effect cannot else be a cause". According to Jawaharlal Nehru[9], in Sankhya System, "The evolution is a continuous thing" and "Causality is accepted but it is said that the effect is really hidden in the cause. Cause and effect become undeveloped and developed state of the same thing."

Perception has been a favourite theme in Indian epistemology[10]. According to Popper[11] "In science, it is observation rather than perception which plays a dominant part". Scientific study of analogous phenomena in physico-chemical systems can serve as a good guide for understandings dynamics of natural systems.

Order, Disorder and Second Law of Thermodynamics

According to Second Law of Thermodynamics, at equilibrium, entropy S is minimum and entropy production dS = 0, while in irreversible processes dS > 0. For any system[12], net entropy production is made up of: i) Internal production in the system d_iS and; ii) Entropy exchanged with surroundings d_eS through exchange of matter or energy or both. Thus

$$dS = d_iS + d_eS \qquad \ldots(1)$$

While d_iS would always be >0, d_eS can be e"0 or <0. In many non-equilibrium systems, specific type of order is developed when there is an appropriate export of entropy to surroundings or environment. However, too much export of entropy by numerous systems can disturb the order and generate disorder in the environment as it has happened in case of global warming due to emission of gases like carbon dioxide (CO_2), methane (CH_4) and chloroflurocarbons (CFC) leading to ozone (O_3) depletion in atmosphere. In such a case, entropy of the environment (d_eS) increases considerably due to import of entropy from specific systems leading to disorder.

There can be following types of systems (Fig. 1): a) Isolated or closed systems where no exchange of matter and energy takes place, and system attains equilibrium state ultimately; b) Systems involving exchange of energy only [These can be of two types: i) Discontinuous {two subsystems separated by a barrier (bio- membrane, where temperature T and pressure P may be different in two chambers but constant in space in each chamber)} and ii) Continuous (T and P change from point to point)]; c) Systems involving exchange of matter and energy such as continuously stirred tank reactor (CSTR); and d) Complex systems with a network of systems such as human body or a continent or globe itself [subsystems can be of type a) or type b)]. Global system consists of earth, the surrounding, atmosphere and O_3 sheath. Internal production of entropy of system d_iS is continuously increasing due to emission of CO_2, CH_4, NO and CFC leading to O_3 depletion. Deforestation is also promoting such a situation. With UV radiations passing through ozone layer, energy is imported from the universe, leading to increase in global entropy dS and thus generating disorders as global warming and unpredictable weather changes.

Causality principle, Non-equilibrium Thermodynamics and Nonlinear Science

Linear and Steady State Phenomenon

Non-equilibrium thermodynamics provides a model framework for providing cause-effect relationship simpler systems involving multiple forces (causes). However, for more complex situations, non-linear dynamics and

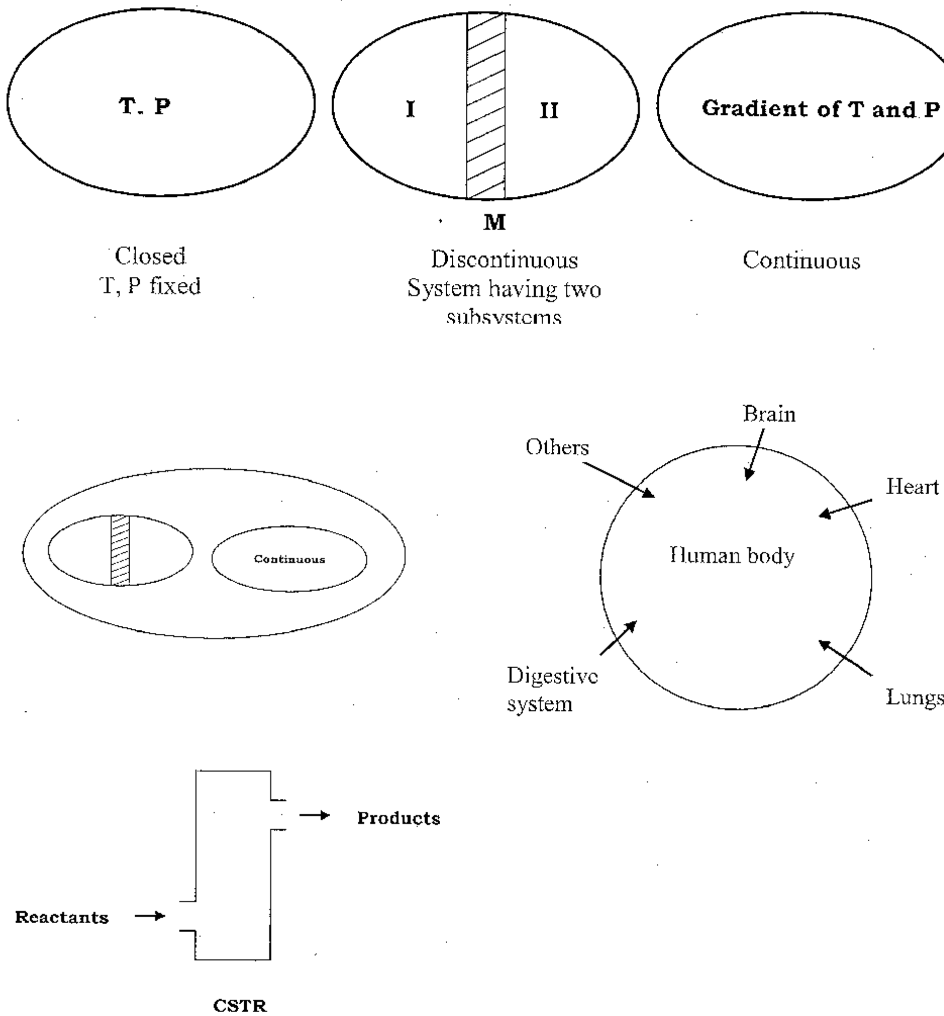

Fig. 1—Some typical systems in nature

computer simulation has to be used in order to supplement basic information.

Single Cause- Effect Phenomena

In this paper, cause & force and effect & flow (flux) would be treated as synonym. Single cause- effect phenomena are well known (Table 1). Causal laws can be represented as

$$J = LX \quad \ldots(2)$$

where X is force, J is flow and L is a constant called phenomenological coefficient (PC). L can depend on other variables[4]. Primary cause is X. However, factors influencing magnitude of L can only affect magnitude of effect. Thus, relation between blood flow and pressure becomes non-linear when radius of capillary increases due to widening of capillaries[4].

Cross-Phenomena and Coupling between Fluxes and Forces

Forces can produce more than one type of effect, when: a) Forces generate same effect, reinforcement of the effect occurs; and b) One or more forces produce opposite effect, in course of time steady state is observed under specific conditions.

One of such typical non-equilibrium phenomena is electro-kinetic phenomena (EKP). Consider a system

Table 1— Single cause-effect phenomena

Phenomena	Cause	Effect	Law
Thermal conduction	Heat flow	Temperature difference	Fourier's Law
Viscous flow	Pressure gradient	Volume flow	Poisseuille's Law
Electrical conductivity	Potential difference	Flow of current	Ohm's Law
Diffusion	Concentration difference	Mass flow	Fick's Law

consisting of two chambers (I and II) containing same specific fluid, separated by a barrier (membrane containing channels of fine pore). Two electrodes inserted in each chamber connect both chambers electrically. When potential difference (primary force) is applied, flow of fluid (electro-osmotic flux) causes build-up of higher pressure in other chamber. Now, pressure difference acts as a secondary force X_1, which generates hydrodynamic flow that pushes fluid in opposite direction. Ultimately, when two flows are balanced, a steady state is obtained and steady electro-osmotic pressure corresponding to fixed pressure difference is developed. Potential difference is designated as X_2. Non-equilibrium thermodynamics[3,4] has been very successful in interpreting such a non-equilibrium phenomenon, which can serve as a model for natural system. Entropy production can be given as

$$d_i\Sigma/dt = \Sigma J_i X_i, (i= 1, 2) \quad ...(3)$$

When no potential difference, but a fixed pressure difference (as primary force) is imposed, electric current (streaming current), which generates corresponding potential difference (secondary force), generates normal current (Ohmic) that flows in opposite direction. Ultimately, a steady state is obtained and a steady potential difference (streaming potential) is maintained. Linear phenomenological relation between fluxes and forces is assumed in NET. So that

$$J_1 = L_{11}X_1 + L_{12}X_2 \quad …(4)$$

$$J_2 = L_{21}X1 + L_{22}X_2 \quad …(5)$$

where J_1 is net fluid flow, J_2 is net current, L_ik are PCs. Here, $L_ik = L_{ki}$ on account of Onsager reciprocity relation. Two steady states are given by

$$(X_1/ X_2) J_2= 0 = - L_{12}/L_{11} \quad …(6)$$

$$(X_2 /X_1) J_1= 0 = - L_{21}/L_{22} \quad …(7)$$

Further, within domain of validity of linear phenomenological equation, entropy production is minimum in steady state. PCs depend on other variables similarly as CC, as demand – supply relationship depend on number of parameters (cost of material, infrastructure, yield, transport arrangement, political situation), which act as causes for influencing magnitude of effect. Studies[4,13] provide adequate justification of linear phenomenological relation, onsager reciprocity relation and two steady state relations.

Non-equilibrium thermodynamics[12,14,15] is a valuable tool where coupling of fluxes and forces are involved. Number of phenomena involving such coupling[4] has been investigated.

Phenomena Involving more than Two Forces

Non-equilibrium thermodynamics is also applicable in systems where coupling between more than two forces is involved. Linear phenomenological equations are given as

$$J_i = \Sigma L_{ik} X_i (i, k = 1,2,……n) \quad ...(8)$$

$$\text{or, } J_1 = L_{11}X_1 + L_{12}X_2 + L_{13} X_3 +…… \quad …(9)$$

$$J_2 = L_{21}X_1 + L_{22}X_2 + L_{23} X_3 +…… \quad …(10)$$

$$J3 = L_{31}X_1 + L_{32}X_2 + L_{33} X_3 + ……. \quad …(11)$$

$$L_{ik} = L_{ki} \quad …(12)$$

Equations were successfully applied to studies[12,14] on: i) EKP involving solutions of non-electrolytes; ii) Thermo-osmotic concentration difference with forces pressure difference ΔP, temperature difference ΔT and concentration difference ΔC; and iii) Thermal diffusion potential.

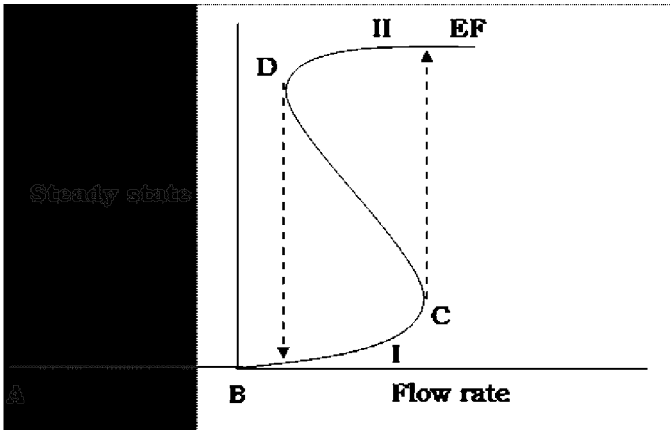

Fig. 2—Biostability in a typical system (C and D are typical bifurcation points)

Approach and Transition from One Steady State to Another

Approach to steady state and transition from one steady state to another is of considerable interest in social sciences and health sciences (transitions from one state to another for disease and subsequent treatment or with age are involved). Build-up of electro-osmotic pressure difference and thermo-osmotic pressure and its approach to steady value and relaxation time have been experimentally estimated[4,16].

Non-Linear Flux Equations and Non-Linear Steady State

Non-equilibrium thermodynamic formalism, only valid in linear range, is still useful in non-linear range, since: i) Fluxes and forces identified through formalism are valid in non-linear range; and ii) Concept related to development of order by export of entropy holds well. Experimentally, non-linear steady states in EKP and chemical reactions in CSTR have been studied[4,17]. However, non-linear flux equations have been investigated in depth only in EKP. Fluxes are functions of forces and relation between these involve higher powers of forces as

$$J = f(X_1, X_2, \ldots\ldots) \qquad \ldots(13)$$

When only two forces are involved, J_1 can be represented as

$$J_1 = L_{11}X_1 + L_{12}X_2 + \tfrac{1}{2}L_{111}X^2_1 + L_{112}X_1X_2 + \tfrac{1}{2}L_{122}X^2_2 + \ldots. \qquad \ldots(14)$$

where L_{111}, L_{112}, L_{222} are higher order coefficients. In EKP, higher order terms in forces occur because first-order cross- PCs, themselves are functions of forces[4]. Higher order terms in forces appear when magnitude of forces is large. Such non-linear relations are also expected to occur in social and natural systems under specific circumstance.

In chemical reactions, rate can be expressed as power series in chemical affinity, which acts as a force[17]. In gaseous systems, non-linear equations for heat and mass transport do not involve higher powers of gradients but instead involve space derivatives of gradients (this may be of relevance for population dynamics).

Steady states are stable even in non-linear range as observed in EKP and chemical reactions in open CSTR. Further, unlike the case of linear steady states, ratio of steady state values of forces is not constant but is a function of forces. Under such circumstances, entropy production cannot be minima as postulated in Linear Non-equilibrium Thermodynamics (LNT).

Exotic Non- equilibrium Phenomena and Non-linear Science

For interpretation of non-equilibrium region, although basic concepts of LNT are useful, but it has to be supplemented by appropriate experimental studies and mathematical analysis involving non-linear dynamics and numerical simulation studies. Non-linear dynamics essentially involves mathematical modeling based on physical mechanism using non-linear algebraic equations (exponential, parabolic), ordinary partial differential equations, integral or a combination of these. Nature of solutions of such equations changes when the value of a certain parameter (bifurcation parameter) changes at a certain point or stage (bifurcation point). In such relations, effect itself acts as cause (prey-predator relation, tree-seed relation or egg-chicken relation). In terminology of chemistry, such relations are called as autocatalytic relation.

Bifurcation Phenomena and Bi-stability

On moving away from equilibrium, scenario follows as: i) Equilibrium state—time-invariant, no forces present; ii) Steady state — time-invariant, forces present; and iii) Bi-stability—time-dependent state, space-dependent. On moving along AB (Fig. 2), system has either to move to state I or II (B is bifurcation point). Further, successive bifurcation can also take place. Considering following mathematical relation

$$x^2 = a \qquad \ldots(15)$$

Which gives, $x = \pm\sqrt{a}$. Bifurcation point occurs at $x = 0$. If one moves from negative values of variable towards positive values of a, one gets two values of x. Successive bifurcations are also possible as it happens in historical evolution or in city's road map.

Away from steady state, in certain cases, a situation may arise when there is a sudden jump from one stable state to another involving hysteresis as it occurs in magnetism. Kinetics of reaction system is governed by flow rate of reactants in CSTR. Steady state changes with flow rate along the curve AB (Fig. 2). When flow rate reaches state B (bifurcation point), there is a sudden transition (jump in the potential) and subsequently state II follows path DF as flow rate is increased. When from point F, flow rate is reversed (decreased), there is a sudden fall from state E to C. Here again sudden bifurcation from bifurcation point E to steady state C occurs.

In order to decipher causal relation for such a phenomenon in case of a reacting system, Schlogel's model is very useful. Considering following set of reactions:

$$A + 2X \rightleftharpoons 3X$$
$$X \rightleftharpoons B$$

where X is intermediate product, which is produced autocatalytically. A is reactant and B is final product. Both are connected to their respective reservoirs so that their concentrations are kept fixed. kms:$_1$ and k_2 are rate constants of the forward and back reactions of first step while k_3 and k_4 are rate constants of second step.

If X_o is steady state value, it is found to depend on $b = k_4 .B / k_2$ and reaction scheme yield a quadratic relation between X_o and b. When X_o is plotted against b, one gets a sigmoid curve with hysteresis[3]. Thus, autocatalytic step plays key role in generating bi-stability in the system. In a similar type of complex reactions, key role is again played by complex reaction steps of similar type as is found in bi-stability observed in iodate-arsenite reaction[18]. Mechanism of bi-stability in cerous–bromate system has been elucidated by Bar-Eli and Noyes[20a], which involves complex reaction network including autocatalysis where effect also acts as cause itself.

In Economics, a bi-stability phenomenon has been observed as follows: a) Low production with high price; or b) High production with low price. In financial management[20b], similar situations arise when: a) Large deviation from annual production with large investment; and b) Small deviation from annual production with large investment.

Bi-stability has relevance in biochemistry, physiology as well as physical sciences as follows: a) Bi-stable behaviour of an animal under stress (fight or flight) in animal psychology, depression and enthusiasm in human psychology; b) Switching mechanism in nerve cells from rest to action potential; epileptic brain, seizure in epilepsy; and c) Bi-stable mechanism in enzyme reaction, protein/biochemical systems.

Transition States: Time-dependent Non-equilibrium States

Simplest time independent state is equilibrium state in a closed system, where opposing effects exhibit microscopic and macroscopic reversibility but forces are non-existent. Other time-invariant state is non-equilibrium steady state in open systems involving two or more forces, where effects of same type are balanced. Time-dependent, space-dependent or space-time-dependent states in open systems often exhibit order and organized pattern[3,4] when entropy exported to the surroundings is positive.

Extensive and comprehensive studies on chemically reacting systems[21-23] have yielded a very clear picture of oscillatory behaviour in closed as well as open systems, knowledge of which would be useful to social sciences and medicinal sciences. Several types of periodic behaviour are (Fig. 3): a) periodic; b) bi-periodic; c) tri-periodic; d) sequential separated by a time-pause; and e) chaotic. Complex oscillations are observed in weather, stock market, price fluctuations, electro-cardiogram (ECG), electro-encephalogram (EEG) and population dynamics.

Prigogine[15] proposed a model multi-component reaction scheme (called 'Brusselator') based on non-linear kinetics, which predicted oscillation on solving non-linear differential equation by computation as

$$A \rightleftharpoons X \quad (S1)$$
$$B + X \rightleftharpoons Y + D \quad (S2)$$
$$Y + 2X \rightleftharpoons 3X \quad (S3)$$
$$X \rightleftharpoons F \quad (S4)$$

Reactants A and B interact to generate species X and Y. Oscillations, controlled by key reactions, involve autocatalysis of X via step S3 simultaneously with its inhibition/destruction via step S4. In step S3, cause X produces itself. Oscillatory reactions have been extensively studied[21-23] and mechanism elucidated. In

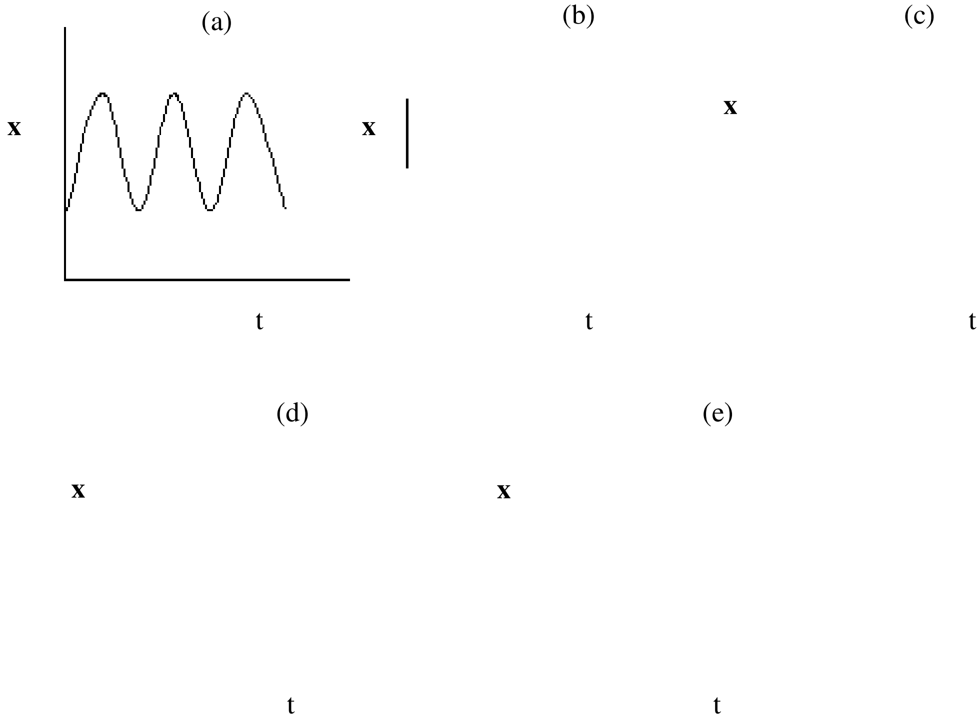

Fig. 3—Periodicity and complex time-series (x = variable, t = time): a) periodic time-series; b) Bi-periodic time-series; c) Tri-periodic time- series; d) Sequential series with a time-pause; and e) Chaotic time-series

this context, mechanism of variants of Belousov-Zabotinskii (B-Z) reaction has been found based on Field-Koros-Noyes (FKN) mechanism as

$A + Y \rightarrow X$ (R1)
$X + Y \rightarrow 2P$ (R2)
$A + X \rightarrow 2X$ (R3)
$2X \rightarrow P + A$ (R4)
$Z \rightarrow fY$ (R5)

where $A = BrO_3^-$, $X = HBrO_2$, $Y = Br^-$, $Z = 2\ Ce_4^+$, P = product (HOBr) and f = constant

Hard core of reaction mechanism is autocatalytic reaction [R3] and inhibitory reaction [R4]. Basic force in chemical reactions is free energy change delta* G during product formation from reactants. For reaction to occur, free energy change has to be negative. Time-order is governed by non-linear dynamics, complexity and oscillatory features that depend on number and concentrations of components and number and nature of steps; control mechanism involves positive feedback (autocatalysis) and negative feedback (inhibitory step), there can be more than one control mechanism depending on number of sets of autocatalytic and inhibitory reaction sets.

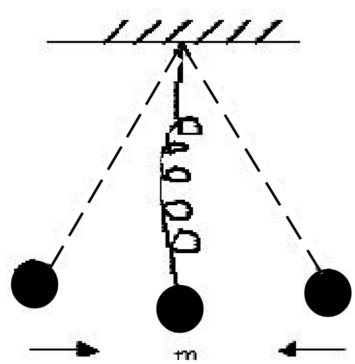

Fig. 4—Simple harmonic motion of pendulum

In case of B-Z reaction systems (malonic acid + potassium bromated + ceric sulphate + sulphuric acid), bromide-ion control mechanism is operative. However, when organic substrate is replaced by fructose, a different mechanism (free-radical control mechanism) operates[24]. On the other hand, when it is replaced by fructose + oxalic acid or glucose + oxalic acid, oscillations are governed by both control mechanisms[25]. Therefore, there is tug of war between opposing forces. Normally, a steady state can be reached, but if there are constant sources of disturbance, periodic or complex periodic variation with time can occur. For example, a pendulum is resisted by the tension F = kx, where k is stiffness and x is displacement in space. Push to pendulum (mass m) along X-axis generates force of acceleration (m.x), which is equal to resultant of gravitational force, and force of restitution acting in opposite direction (Fig 4). This leads to differential equation for simple harmonic motion (periodic oscillations) governed as

$$m.d^2x / dt^2 = -kx \quad ....(16)$$

Simple periodicity is very often not observed in nature. Typical non-periodic situations occur in economics and human physiology. Electric potential oscillations at solid-liquid, liquid-liquid and liquid-vapour interface are analogues of oscillations involved in membranes and sensing mechanism of taste and smell[4,13] where mathematical modeling has been attempted using Van der waals equation as

$$m.d^2x/ dt^2 + p.dx/dt + kx = 0 \quad ...(17)$$

Time-delay equations have also been used to predict oscillations in economics[4]. In economics and finance, non-periodicity is too common; even chaos has been noted. Chaos, which can be predicted mathematically, is called deterministic chaos. Lorentz' oscillator[26] predict uncertain weather changes successfully as

$$dx/dt = -\sigma x + \sigma y \quad ...(18)$$

$$dy/dt = xy + r.x - y \quad ...(19)$$

$$dz/dt = xy - bz \quad ...(20)$$

where, σ , r and b are constants. Here x is produced by y and y is produced by x. Together, x and y constitute a cross-catalytic subset (for positive feedback).

In many cases, periodicity is disturbed by noise, which in chemical systems can result from experimental noise, local inhomogeneity resulting from gas bubbles or mixing effects or gas evolution in heterogeneous reactions[27]. In socio-political or socio-economic systems, this can result from small disturbances by external forces. In nature as well as in living or social systems, role of coupled oscillators can be significant[4]. These may be physically coupled in social systems, while in chemical systems these can be coupled chemically or both chemically and physically.

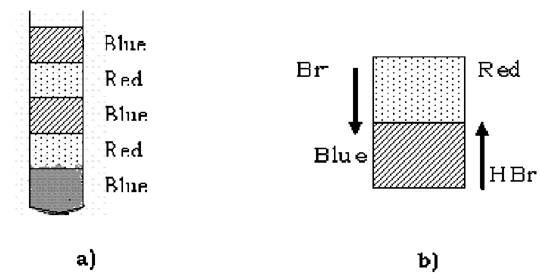

Fig. 5—Spatio-temporal oscillations (chemical waves): a) Pattern; and b) Diffusion of chemical species

Non-equilibrium Space-dependent States

In non-equilibrium states, situations can be noticed when variability is observed from point to point in space. Typical example is population distribution in a country, where population density variation occurs with time and also with respect to region. Another example is pattern formation on tiger skin. Spatio-temporal oscillations in physico-chemical system provide a basis for understanding such phenomena, which are governed by chemical reactions and diffusion.

Chemical waves are produced when B-Z reaction mixture along with phenanthroline as indicator is taken in a test tube. Initially, colour of solution becomes red. Chemical wave proceeds from bottom. Blue band, formed at the bottom, is followed by a red band, the cycle is repeated and a moving banded structure (Fig. 5a) is formed. Here, system is open, is in non-equilibrium state and generates oscillations with time as well as periodic variation in space.

Oscillations are governed by control mechanism, as in B-Z systems. Wave movement, which is governed by diffusion of some specific species, is responsible for dissipation of entropy and emergence of an organized pattern in space. Concentration of Br- decreases in beginning below a critical value, when blue-coloured reaction wave starts from the bottom. Oxidation stage takes place and leading edge of wave (sharp blue boundary) with high [$HBrO_2$], [Fe^{3+}] and low [Br^-] is formed. Diffusion of $HBrO_2$ occurs from blue zone to red while diffusion of Br^- occurs from red zone to blue yielding an organized pattern (Fig. 5b). Change in concentration due to diffusion of particular reactant A is governed by Fick' second law of diffusion as

$$dC_A / dt = D_A \, d^2C_A /dx^2 \quad ...(21)$$

Whereas rate of concentration change due reaction is given as

$$dC_A /dt = f (C_A,C_B,\ldots\ldots..) \quad \ldots(22)$$

where A, B,…. are reactants. Dynamics of wave propagation and change in concentration of a particular species is governed by Reaction-Diffusion equation[21,22] (non-linear) as

$$dC_A/dt = D_A\, d^2C_A /dx^2 + f (C_A,C_B,\ldots\ldots.) \quad ...(23)$$

where D_A denotes diffusion coefficient of species A. In case of wave propagation in B-Z system, following expression for wave velocity V is obtained:

$$V = \sqrt{(4D_A k_5[H^+][BrO_3^-]C_A} \quad \ldots(24)$$

where k_5 is rate constant of step 5 of FKN mechanism, which involves destruction of bromous acid[4]. In other words, wave velocity is proportional to square root of $[H^+]$ and $[BrO_3$-].

Another type of space structure, Leisegang rings[4] is obtained when a specific reactant B is added to solution of A in gel. Two reactants diffuse from opposite directions and co-exist in gel until solubility product reaches a critical value above following reaction takes place leading to the formation of precipitate (product C) and subsequent nucleation to form crystal as

$$A + B \rightarrow C \rightarrow \text{Nuclei} \rightarrow \text{Crystal}$$

Once nucleation starts, depletion of concentration of A and B occurs in surroundings. Hence a stage comes, when precipitate formation stops and clear space is formed. Nevertheless, diffusion of ions persists and nucleation and subsequent precipitation takes place beyond clear space. Process is repeated and a banded structure (precipitate/ clear space) is formed.

Complicated spatial structures that result depending on experimental conditions[4,28] are: i) Three-dimensional patterns; ii) Quasi-two-dimensional structures in CIMA reaction[28]; iii) Hexagon stripes; iv) Black-eye pattern; and v) Dividing bulbs, chemical flowers and patterned islands. Such non-equilibrium patterns are observed in social systems, demography and living state, due to involvement of multiple causes and processes. In population dynamics, diffusion plays a significant role depending on job-facility, business facility and infrastructure.

Fig. 6—Typical fractal pattern: Contour set

Irregular Spatial Patterns in Nature and Fractal Geometry

Typical examples of irregular geometry are clouds, and coastline of England and Norway. Similar examples have been observed in physico-chemical systems such as crystal growth, bacterial growth and electro-deposition[4]. Normal concept of spatial order is based on Euclidean geometry. Recent developments in fractal geometry[29a] structures possess an order defined by fractal dimensions in contrast to Euclidean dimension in integral numbers. Further, comprehensive studies have been undertaken to elucidate mechanism of fractal growth, which involves diffusion-limited -aggregation[29b]. Fractal geometry language has been used to have an insight into different types of non-equilibrium growth processes. Fractals[30] look more or less similar on many scales of magnification.

Self-similarity of objects can be analyzed, using concept of fractal geometry. Self-similar objects can be divided into N parts (subunits) of length l. For example, in Contour set. (Fig. 6), take a line A. In case a), cut this line into three equal parts and generate two subunits with vacant space in the middle. In case b), again cut two pieces in a) in three parts and generate four subunits. Further in case c), again cut four pieces into three parts of b) and generate eight subunits. Go on repeating the process again and again. Resulting arrangement would be self-similar. Evidently, dimension of such a structure cannot be put equal to one (Euclidean dimension for line A). Now, fractal geometry provides a procedure for evaluation dimension in above case, which is fractional. Fractal dimension D is given as

$$D = \ln N/ \ln n \quad \ldots(25)$$

where, N = number of subunits and n is number of parts. Therefore, for above case

$$D = \ln 2 / \ln 3 = 0.6309 \text{ (fraction not an integer)} \quad \ldots(26)$$

Fractal dimensions have been estimated for more complex structures by identifying basic features of self-similarity. Fractal dimensions of some natural objects are as follows: Coastline of Norway, 1.5; retina, 1.7; *Bacillus subtilis*, 1.7; and *Escherchia coli*, 1.5.

Mathematical techniques involving probability statistics (sticking probability) along with computational techniques, which have been utilized to theoretically compute fractal dimensions, satisfactorily agree with experimental values. Concepts based on fractal geometry and growth, are of considerable value in archaelogy[31], town planning and urban development.

Determinism and Social Organization

Recent developments in scientific studies of non-equilibrium phenomena can serve as a useful guide for analysis of similar phenomena in social and natural systems. Bifurcation from one steady state to another can occur in three ways: i) Since there are external variables or secondary forces, which can affect CCs, thereby leading to attainment of a different steady state, which would involve a certain relaxation time; ii) If by some mechanism, magnitude of forces is altered, another steady state would be attained also requiring adequate relaxation time; and iii) A situation may arise, when on changing a particular variable, sudden bifurcation to either of the two steady states at a particular bifurcation point, may occur. In historical evolution and development of social organization and social psychology or even in the context of stability of steady state in human physiology, attainment of steady states after transitions is an important feature, which leads to so-called self-organization or self-adjustment.

So far time-invariant state in the context of cause-effect relationship had been considered. Periodic changes in time and space are also a common feature in natural systems. Just as a slight disturbance to pendulum generates simple harmonic motion, similarly a disturbance due to a particular type of force can initiate oscillations in a typical steady state. For example, in the case of EKP, where steady states are obtained due to opposing effects of potential difference and pressure difference, steady state can be disturbed by concentration difference yielding periodicity in time. However, in such a case, equation for simple harmonic oscillations is not adequate. On the other hand, Van der Waal equation for non-linear oscillations has to be used. Non-linear dynamics based on non-linear equation has been successfully used for the interpretation of similar type of phenomena, as seen in the case of oscillatory phenomena at different types of interfaces.

Studies on oscillatory chemical reactions in CSTR, which is an open system, reveal importance of autocatalytic reaction (positive feedback) and inhibitory reaction (negative feedback). In population dynamics, living species themselves multiply providing example of autocatalysis. Similarly, corruption breeds corruption and bad governance leads to worse governance as is observed in under-developed or developing countries. Thus, type of mechanism is quite relevant for social systems. Time-delay equations have also been invoked in modeling time-periodicity in economics and human physiology.

Weather changes are sometimes unpredictable and mathematical formalism can predict chaotic conditions in weather (Deterministic chaos). However, unpredictability is related to noise caused by external factors such as global warming. In evolution of societies, diffusion-controlled aggregation is common feature. Sattelite pictures of cities like London and Kolkata clearly indicate fractal growth. Similarly, population density can vary from point to point. In human physiology, network of blood vessels provides example of a fractal structure.

Causal Relations and Predictability

For good governance and decision-making, identification of cause and qualitative relation between cause and effect is vital. In economics and social systems, very often a quantitative relation is needed. Statistical data and mathematical modeling gives useful hints. Experimental verification is possible in physical and biological sciences. Even for medical sciences, *in vivo* and *in vitro* experiments provide useful information. Several features of causal relations are: a) A causal relation between function of one variable (cause) and other variable (effect); b) Statistically, observational studies can give only indication of possible cause and effect; c) As stated by Van't Hoff, Noble Laureate, that " in the mechanism of investigating a causal connection, imagination is necessary in five operations [i) in choice of moment or object of observation, ii) in discretionary alteration of observed, iii) in finding of aids, which facilitate observation, iv) in observation of a correspondence or a dissimilarity and v) in setting up a hypothesis]"; and d) Mathematical modeling and non-linear analysis to a certain extent can be useful in predicting causality relation.

Social psychology significantly influences socio-political and socio-economic systems. Three types of social psyche[32] (tendencies) are prevalent and co-exist in such systems as follows: 1) Sattvik - Free from attachment, unegoistic, endowed with firmness and vigour and unswayed by success or failure; 2) Rajsik – Doer, who is full of attachment, seeks fruit of actions and is greedy, and who is oppressive by nature and of impure conduct, and is affected by joy and sorrow; and 3) Tamsik - Lacking piety and self-control, uncultured, arrogant, deceitful, inclined to rob others of their livelihood, slothful, down-hearted and procrastinating. Dynamics of changes in social psychology in the context of attitude and temperament undergo transitions in the following sequence according to Indian Philosophy : Enhancement of ethical values in the society $\rightarrow$S (Sattvik) $\rightarrow$R (Rajsik) $\rightarrow$T (Tamsik) $\rightarrow$Chaos, whereas, first stage is a slow process, second and third stages are autocatalytic. After third stage, chaotic conditions can prevail. Only when disorganization goes to extreme limit, intolerable to society, first stage again becomes active and cycle repeats again and again. Philosophy, ethics and social psychiatry have been clearly discussed in Gita[32], which basically involves philosophy propagated in Vedas that present views of Indian philosophers and thinkers.

Above sequence is responsible for upheavals both in underdeveloped and developed societies. Stages two and three appear as autocatalytic generation of corruption and mismanagement in underdeveloped societies. This is also true for developed societies, but these tendencies are modified in a more polished form in the shape of industrialization, colonization and world wars. S (Sattvik) in an enlightened form is reflected in League of Nations and UNO. Situation is getting more and more complicated as social, political and economic systems are getting more and more open due to globalization and fast development in communication technology. Consequently, duration of steady state in such systems is diminishing very rapidly.

Unpredictability surfaces when autocatalytic processes are involved in a particular situation as is observed in physico-chemical systems. However, in cases like bi-stability, temporal oscillations and spatio-temporal oscillations, there is possibility of predictability.

Similar type of processes and situations also play an important role in historical evolution. Stability of steady states, transition from one steady state to another and time of relaxation are governed by similar type of considerations. Stability of health depends on life-style. In old age, destabilization of steady state is quite common and occurs more readily as compared to younger age. However, by controlling life-style, it is possible to maintain stability. Shock of death or major incident destabilizes system temporarily. Proper understanding of real causes and cause-effect relationship is also useful in decision-making and management science.

Conclusions

With recent advances in non-linear science and on account of recent theoretical and experimental studies of non-equilibrium physico-chemical systems, capability to predict exotic phenomena like bi-stability, time-order, and space order has advanced considerably. On account of these developments, it is possible to have an idea of causal relations in such situations, both qualitatively and quantitatively. Life is a stimulus-response phenomenon[33]. Social life and social evolution are also similar phenomena leading to frequent self-organization. Any open system undergoes changes when: i) Magnitude of cause changes; ii) Magnitude of correlation coefficient changes; or iii) When new causal factors appear. System takes its own time for adjustment, which involves proper balancing of forces (causes) and fluxes (effect). However, new challenges are emerging, as the global systems are getting more and more open.

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