

Disipation Functions of Flow Equations in Models of Complex Systems

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Abstract In an open system, each disequilibrium causes a force. Each force causes a flow process, these being represented by a flow variable formally written as an equation called flow equation, and if each flow tends to equilibrate the system, these equations mathematically represent the tendency to that equilibrium. In this paper, the authors, based on the concepts of forces and conjugated fluxes and dissipation function developed by Onsager and Prigogine, they expose the following hypothesis: Is replaced in Prigogine's Theorem the flow by its equation or by a "flow orbital" considering conjugate force as a gradient. This allows to obtain a dissipation function for each flow equation and a function of orbital dissipation.

Keywords: conjugate forces, dissipation function, equilibrium, flow equations, flow process, flow orbital, synonymous equations

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1. Introduction

For the General Systems Theory, the concept of order is a relative concept. The essence of the system is always an ordination class. In general, the subject conceived as order, that which harmonizes with their cognitive processes, produced by the dilemma of whether it refers to a state S of System H or Subject's capacity as observer to recognize it. One thing in itself means nothing. It is the relationship of the subject with it which gives meaning. Therefore, *disorder*, that is, the total absence of any kind of order, not have any logical significance. To say that a system H is disordered means that *the subject does not have sufficient information to specify in what order is*. In the words of the Mathematical Theory of Information (Shannon, 1948), one could say that entropy measures how much information the subject needs to understand what is the order that has a system that, for the moment, it seems messy. The *difference or similarity* leading to order are concepts prior to its own idea.

The type of equilibrium that reaches the H system and its maintenance depends heavily on its relationship with H' and H" (environmental stimulus and response respectively). Systems do not suffer processes but are the forms taken by the processes as they are only abstractions in the mind of the subject of what remains relatively constant in a process of movement and transformation. *There is no permanent system*. There are processes obviously being irreversible, which constitute the history of the H system, involving changes in structure and information. That is, H carries its own story in the form of structure and "altered" function with respect to which

possess "if it had not happened." In system H, the past is assimilated into the memory structure. The subject follows the processes by observing the structure, which is nothing more than a stage in the space-time continuum. Complex structural causal systems, are not balanced systems and therefore, the processes are not balanced in turn.

Consider a system $H[t_0, t]$ consisting of two states $S_1[t_0, t], S_2[t_0, t]$. Consider that states are given the probability distributions $S_1[t_0, t], S_2[t_0, t]$ found with energies E_i^1, E_i^2 that are p_i^1, p_i^2 . The corresponding entropies are:

$$\Sigma_1 = -k \sum_i p_i^1 \log p_i^1 \quad \Sigma_2 = -k \sum_i p_i^2 \log p_i^2 \quad (1)$$

where K is the Boltzmann constant. The energies are:

$$E^1 = \sum_i p_i^1 E_i^1, \quad E^2 = \sum_i p_i^2 E_i^2 \quad (2)$$

Considering the sum of constant energy:

$$E^1 + E^2 = E \quad (3)$$

The entropy is additive:

$$\Sigma^1 + \Sigma^2 = \Sigma \quad (4)$$

Therefore:

$$\frac{\partial \Sigma}{\partial E^1} = \frac{\partial \Sigma^1}{\partial E^1} + \frac{\partial \Sigma^2}{\partial E^1} = \frac{\partial \Sigma^1}{\partial E^1} + \frac{\partial \Sigma^2}{\partial (E - E^2)} = \frac{\partial \Sigma^1}{\partial E^1} - \frac{\partial \Sigma^2}{\partial E^2} \quad (5)$$

and in accordance with the thermodynamics (Jou & Llebot, 1989; Volkenshtein, 1981)

$$\frac{\partial \Sigma}{\partial E^1} = k(\beta^1 - \beta^2) = \frac{1}{T^1} - \frac{1}{T^2} \quad (6)$$

being β^1, β^2 two undetermined Lagrange multipliers and T^1, T^2 the temperatures of states. If the system is not balanced, facilities, including entropy, are time dependent. During the contact of two states, having, for example, different temperatures, elapses the transfer of any physical quantity including, for example, energy.

2. Flow Process

We define flow process, as the movement of matter or energy between stimulus environment H' and states of system H, among these, or between those states and response environment H''. Therefore, a process flow is necessarily response, transition, internal transition, or internal response, but not in the reverse case. Any kind of these processes need not necessarily be a flow process.

2.1. Dissipative Function in Flow Processes

Due to this displacement, probability distributions will change as follows:

$$\Sigma[t_0, t] = -K \sum_i p_i[t_0, t] \log p_i[t_0, t] \quad (7)$$

In the case of a flow of energy

$$\frac{d\Sigma}{dt} = \frac{d\Sigma}{d\Sigma^1} \frac{d\Sigma^1}{dt} = \left(\frac{1}{T^1} - \frac{1}{T^2} \right) \frac{d\Sigma^1}{dt} \quad (8)$$

The general process of flow of energy is given by the following formula:

$$P_{E^1} = \frac{dE^1}{dt} \quad (9)$$

And there exists a generalized force associated with the flow process, which is given by:

$$\bar{F}_{E^1} = \frac{1}{T^1} - \frac{1}{T^2} \quad (10)$$

Any process flow for a energetic or material variable X,

$$\begin{aligned} X[t_0, t] &\in Z[t_0, t] \wedge X[t_0, t] S[t_0, t] \wedge X[t_0, t] Y[t_0, t] \\ [t_0, t] &\subset T, t_0 < t \quad P_\Psi(X[t_0, t]) \end{aligned}$$

implies the existence of one or more *conjugated forces* $\bar{F}(X[t_0, t])$ whose mission is to change the structure. Without the existence of $\bar{F}(X[t_0, t])$ does not exist $P_\Psi(X[t_0, t])$. There is a relationship between $P_\Psi(X[t_0, t])$ and $\bar{F}(X[t_0, t])$. A gradient Δ between two points appears, said gradient decreases as time passes, resulting $P_\Psi(X[t_0, t])$ in increasingly lower. Annulled $\bar{F}(X[t_0, t])$, disappears $P_\Psi(X[t_0, t])$. The balance will be restored. If the gradients are small, the processes are acceptably linear. For large gradients, the relationship between flows and forces, ceases to be linear. Physically,

large gradient means large imbalance, and conversely, if the gradients are small, the relations between flows and forces tend to be linear. *Each imbalance creates a force, each force causes a flow and each flow tends to balance the system.*

A flow depends not only on its conjugate force but that can depend on any other force present in the system, which in turn is the conjugate force to some other flow. When the balance is disturbed because an imbalance between two or more points in the system appears, are originated many flows, which tend to restore balance to the system, and these flows are not entirely independent of each other, because in principle, all these flows and associated forces are related.

If the system is characterized by the existence of many variables, the entropy change in time is represented as a sum of products of generalized flows, and the forces conjugate to these flows:

$$\frac{d\Sigma}{dt} = \sum_i P_\Psi(X[t_0, t]) \cdot \bar{F}(X[t_0, t]) \quad (11)$$

The entropy change in the system H is composed of entropy production $d_H \Sigma$ within system H, entropy flow $d_H \Sigma$ from the stimulus environment H' and entropy flow $d_H \Sigma$ that goes from system H to the response environment H''. Therefore:

$$d\Sigma = d_H \Sigma + d_H \Sigma + d_H \Sigma \quad (12)$$

According to the second law of thermodynamics $d_H \Sigma \geq 0$, and not being given the signs of $d_H \Sigma$ and $d_H \Sigma$. In case that H is a closed system, that is, when only have internal transition processes $d_H \Sigma + d_H \Sigma = 0 \Rightarrow d_H \Sigma = -d_H \Sigma$, and therefore $d\Sigma = d_H \Sigma$. That is, entropy is produced by the energy-material exchange between two states of the state space of H and as a result, sooner or later an energy-material balance is restored. In this case, and only in this, the equation (11) represents the call *Prigogine dissipation function* that is represented by σ . That is, this function represents the rate of production of entropy per unit volume dV .

According to the second law of thermodynamics:

$$\frac{d_H \Sigma}{dt} = \int \sigma \cdot dV \geq 0 \quad (13)$$

and according to (11):

$$\sigma = \sum_i P_\Psi(X[t_0, t]) \cdot \bar{F}(X[t_0, t]) \quad (14)$$

being $P_\Psi(X[t_0, t])$ internal transition processes.

Prigogine (1955) postulated that if external forces acting on the system are held constant and the imbalance that occurs in the system is small, so that the relationship between the flow $P_\Psi(X[t_0, t])$ and conjugate force $\bar{F}(X[t_0, t])$ is linear, H tends to a steady state in which the entropy production is minimal. However, we can say the following:

1. Validity of this principle is restricted if and only if H is a closed system. Can be abstracted and considered initially approaches to Prigogine's principle obviating the presence of H 'and H".

2. If H is a closed system, the validity of this principle has a second constraint: be valid only for situations close to equilibrium. When processes are away too, a crisis is reached and the system structure changes.

3. In complex systems (ecological, socio-economic, etc.), the relationship between $P_{\Psi}(X[t_0,t])$ and $\bar{F}(X[t_0,t])$ is not linear as required by the principle of Prigogine.

4. There are situations where even though the system is continuously organized, a continuous increase is observed in the production of entropy. These are situations in which H does not tend to minimize σ .

2.2. Conjugation of Flows and Generalized Forces

Generalized flows $P_{\Psi}(X[t_0,t])$ depend on the generalized forces $\bar{F}(X[t_0,t])$ and vice versa. In a case of a social model of demographic type, flows of increase or decrease of a population depend on the differences, or gradients of population. In the case of a bioenergetics model, the flows of energy depend on energy gradients and whether the biogeochemical model, flows of matter depend on the concentration gradients (Jorgensen, 1988). In the ideal case of a closed system and with linear approximation

$$P_{\Psi_i}(X[t_0,t]) = \sum_{j=1}^n L_{ij} \cdot \bar{F}_j(X[t_0,t]) \quad (15)$$

being L_{ij} the phenomenological coefficients. In the vicinity of equilibrium in a closed system, and according to Onsager's Theorem (Volkenshtein, 1981), the phenomenological coefficients form a symmetric matrix, ie $L_{ij} = L_{ji}$.

Let us assume the case formed by a state and two flows $P_{\Psi_1}(X[t_0,t]), P_{\Psi_2}(X[t_0,t])$, with two conjugate forces $\bar{F}_1(X[t_0,t]), \bar{F}_2(X[t_0,t])$. then:

$$\left. \begin{aligned} P_{\Psi_1}(X[t_0,t]) &= L_{11}\bar{F}_1(X[t_0,t]) + L_{12}\bar{F}_2(X[t_0,t]) \\ P_{\Psi_2}(X[t_0,t]) &= L_{21}\bar{F}_1(X[t_0,t]) + L_{22}\bar{F}_2(X[t_0,t]) \end{aligned} \right\} \quad (16)$$

According to (15) then:

$$\begin{aligned} \sigma &= L_{11}\bar{F}_1^2(X[t_0,t]) \\ &+ (L_{12} + L_{21})\bar{F}_1(X[t_0,t])\bar{F}_2(X[t_0,t]) \\ &+ L_{22}\bar{F}_2^2(X[t_0,t]) \geq 0 \end{aligned} \quad (17)$$

Dissipation function σ is positive for whatever the nonzero values of conjugate forces and vanishes only if $\bar{F}_1(X[t_0,t]) = \bar{F}_2(X[t_0,t]) = 0$. Therefore:

$$\left. \begin{aligned} L_{11} &> 0 \\ L_{22} &> 0 \end{aligned} \right\} \quad (18)$$

and

$$(L_{12} + L_{21})^2 < 4L_{11}L_{22} \quad (19)$$

As the phenomenological coefficients are symmetrical:

$$L_{12}^2 \leq L_{11}L_{22} \quad (20)$$

The sign of the non-diagonal coefficient L_{12} can be any. In the general case

$$L_{jj} > 0, \quad L_{ii}L_{jj} > L_{ij}^2 \quad (21)$$

Condition $\sigma \geq 0$ relates entirely to the sum $\sum_i F_i[X[t_0,t]]P_{\Psi_i}[X[t_0,t]]$, as individual members of it can be negative. This means that there cannot be flow $P_{\Psi_i}[X[t_0,t]]$ separately since $F_i[X[t_0,t]]P_{\Psi_i}[X[t_0,t]] < 0$. In other words, it would mean that the flow would contradict the Second Law of Thermodynamics. However, due to the conjugation with other flow processes have positive values in the open system $F_j[X[t_0,t]]P_{\Psi_j}[X[t_0,t]] > 0$, such flow may inconceivable in the closed system. Only the condition must be fulfilled:

$$\sum_{j \neq i} F_j[X[t_0,t]]P_{\Psi_j}[X[t_0,t]] > |F_i[X[t_0,t]]P_{\Psi_i}[X[t_0,t]]| \quad (22)$$

Thermodynamically, the entropy production in an open or semi-open system, in principle, ensures the existence of processes that are impossible in closed systems. Fluxes $P_{\Psi_i}[X[t_0,t]]$ and conjugate forces $F_i[X[t_0,t]]$ can be both scalar and vector.

2.3. Flow Variable and Flow Equation

Let us assume a causal system, modeled by a set of ordinary differential equations $\{y'_i\}_{i=1}^n$ representing the states of H and therefore is called *state equations*. If $y'_i = f(\Psi_{i1}, \Psi_{i2}, \dots, \Psi_{in})$ to variables $\{\Psi_{ij}\}_j$ are designated *flow variables* (Forrester, 1961; Usó-Domènech et al, 1995, 1997^a) and represent in mathematical symbolic language, a flow process. In turn, each flow variable depends on a set of variables, namely:

$$\Psi_{ij} = F(\phi_1, \phi_2, \dots, \phi_n) \quad (23)$$

This equation Ψ_{ij} for the dependence of the flow variable respect to other variables of system H, is called *flow equation* and variables $\phi_1, \phi_2, \dots, \phi_n$ are called *generating variables of flow equation*. Therefore, any flow process $P_{\Psi}[X[t_0,t]]$ will be represented mathematically in the form of flow equation in the manner expressed in (23). Likewise, the conjugate force $F[X[t_0,t]]$ will be represented as a gradient $\Delta(X)$. It follows that equation (15) is expressed as

$$\Psi_i(X) = \sum_{j=1}^n L_{ij} \cdot \Delta_j(X) \quad (24)$$

and Prigogine's theorem (14) take the form

$$\sigma_{\Psi} = \sum_i \Psi(X) \cdot \Delta(X) \quad (25)$$

σ_{Ψ} being dissipation function of the flow equations.

In particular, for any flow P_{Ψ_i} ($i = 1, \dots, n$ flows of energy-material magnitude X), the dissipation function of flow equation that represents it, is expressed as

$$\sigma_i = \Psi_i(X) \cdot \Delta_i(X); i = 1, \dots, n \quad (26)$$

2.4. Synonymy Relation in Flow Equations

Let $P_{\Psi} [X [t_0, t]]$ be a given flow process of an energy-material variable X , defined on a system H . It is assumed that this process can be defined by w flow equations $\Psi_{\alpha}(X), \Psi_{\beta}(X), \dots, \Psi_{\omega}(X)$ (Usó-Domènech et al, 1995, 1997^b, 2000; Villacampa et al. 1999). We can define the following relationship: $\Psi_i(X)$ and $\Psi_j(X)$ are *synonymous flow equations* $\Psi_i(X)S\Psi_j(X)$, if they describe the same flow process $P_{\Psi} [X [t_0, t]]$.

Usó-Domènech et al., (1997^b) and Villacampa et al., (2000) demonstrate the existence of an equivalence relation on the relationship of synonymy S , and therefore an equivalence class C .

1. Two equations of the same flow process, $P_{\Psi} [X [t_0, t]]$, $\Psi_i(X)$ and $\Psi_j(X)$ are *intrinsic synonymous flow equations* $\Psi_i(X)S_{int}\Psi_j(X)$ if its respective generating variables are the same, changing only at least one of their transformed functions (Usó-Domènech et al., 1995, 1997^{a,b}, 2000) and equation has the same number of elements.

2. Two equations of the same flow process, $P_{\Psi} [X [t_0, t]]$, $\Psi_i(X)$ and $\Psi_j(X)$ are *lengthened synonymous intrinsic flow equations* $\Psi_i(X)S_{eint}\Psi_j(X)$ if its respective generating variables are the same, changing only at least one of their transformed functions not having the same number of elements in the equation.

3. Two equations of the same flow process, $P_{\Psi} [X [t_0, t]]$, $\Psi_i(X)$ and $\Psi_j(X)$ are *extrinsic synonymous flow equations* $\Psi_i(X)S_{ext}\Psi_j(X)$ if their respective generating variables are different, regardless of whether they have the same number of elements the flow equation

2.5. The Generative Grammar G_F

Let us consider a set of primitive p -symbols or variables. Consider the vocabulary developed by the GT grammar and denote by ρ the corresponding symbols of the vocabulary. Then we define the grammar of the flow equations in the following terms:

a) Initial symbol: Ψ

b) *Terminal vocabulary*: defined by the vocabularies associated to the group of considered variables $\{V_{x_i}\} = \{\rho_{x_i}^i, \rho_{x_i}^j, \dots\}$.

c) *Auxiliar vocabulary*: defined by $\{\Psi_i\}_{i=1,2,\dots,n}$, with the mathematical operations $\otimes = \{+, -, \cdot, /$.

d) *Grammar rules*: they define the composition to generate the words and flow equations (sentences). In

Figure 1 it is shown the corresponding developed rules.

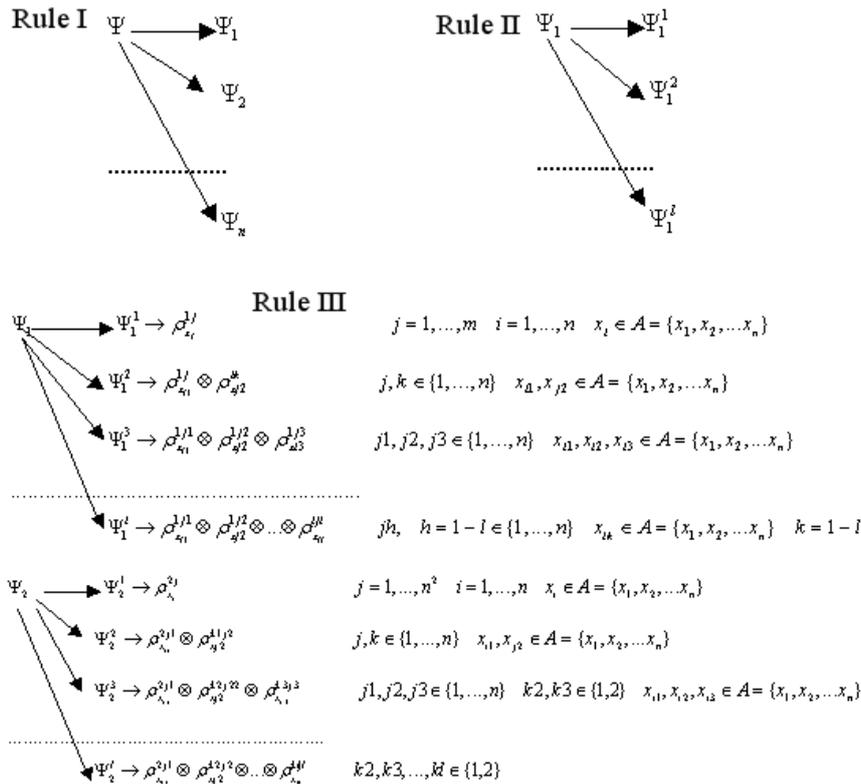


Figure 1. Rules for the generative grammar of flow equations

The GF grammar will generate the L(GF) language or the language of flow equations. The L(GF) language is a formal language because of the following properties:

a) There exists primitive symbols (vocabularies of the variables or lexicon).

There exist complex expressions or formulas (flow equations)

$$\Psi = \rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_n.$$

Each word is a consequence of one or more symbols (combination process).

It is also easy to demonstrate that GF is a non-reductive and free-context grammar (Gladkij and Mel'Cuk, 1972). It is possible to generate words (chains) in this grammar with the property of derivability

2.6. Orbital of Determination of Flow Equations

The same flow process $P_\Psi [X [t_0, t]]$ may be defined by a set of intrinsic synonymous flow equations

$\{\Psi_i(X)\}; i=1, \dots, n$. This set, generated by generative grammar G_F will have equiprobability condition in each of its elements, when they are generated. The number flow equations of set, denoted q , depend of modeler and experimental data. Thereafter, is generated a recogniscibility process, in which a small number of flow equations (w) will be accepted in terms of their "correction". The rest of them, $q-w$, be "wrong". Therefore, we can establish the following criteria for recognizability (Usó-Domènech et al., 1999^a; Villacampa and Usó-Domènech, 1999^{a,b}; Villacampa et al., 1999^{a,b}):

1) RG_{F1} criteria, called the maximum adjustment, based on the statistical coefficient of determination (Usó-Domènech et al., 1997^{a,b}; Villacampa et al., 1999^a). Through an iterative process of searching for the "best" fit of the experimental data from a set of equiprobable flow equations. If it has come to an equation $\Psi_1(X) \in \{\Psi_i(X)\}$ with a coefficient of determination r_1 , may be always find another flow equation whose coefficient of determination is r_2 , with $r_2 > r_1$. The diagram of the recogniscitive process RG_{F1} is shown in Figure 2.

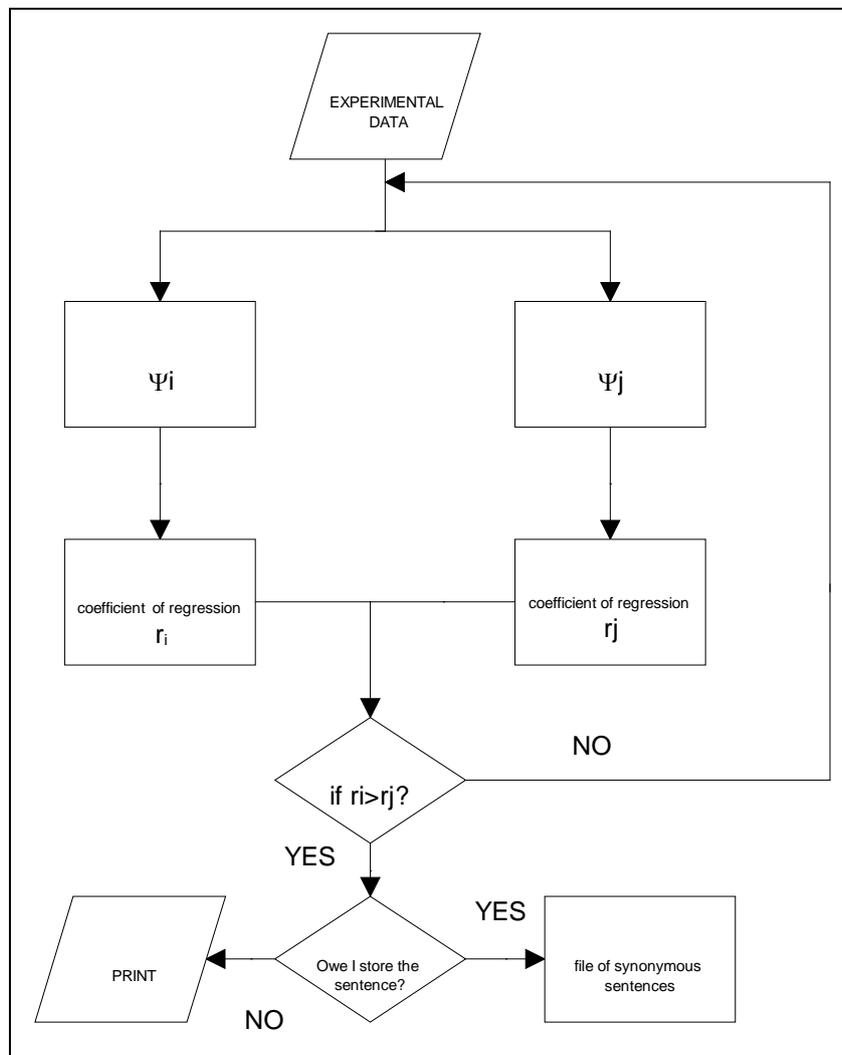


Figure 2. The recogniscitive process RG_{F1}

2) RG_{F2} criteria, defined by the following algorithm: the determination coefficients r_1, r_2 are fixed. There will be a subset of $\{\Psi_i(X)\}$ consisting by all flow equations with coefficients $r_1 \in [r_1, r_2]$, that we will consider as

"correct". This subset will be a subset of probabilistic equations of flow, denominated as *flow equations orbital* or *flow orbital* simply (Usó-Domènech et al., 1997^b) and denote by $\{\Psi_i(X)\}^* \subset \{\Psi_i(X)\}$. Based on the state

equations, we define here three different processes of recognoscibility.

1. A first process of recognoscibility, denoted by RG_{S_1} , is determined by the conception of the model itself.

2. A second process of recognoscibility, denoted by RG_{S_2} , is independent from the first one and determines if

the sentences A_j in $\frac{dy_j}{dt} = \sum_{i=1}^n x_{ij}; j=1,2,\dots,n$, are

“correct” or not where every Ψ_i corresponds to a flow equation. Then, we have several possibilities:

2a) We fix the words and sentences and if any word is correct, the sentence will also be. This kind of recognoscibility process is determined by the validation process. This confirms and reinforces Jorgensen (1988) when he says that validation is always required.

Attempt should be made to get data for validation which are entirely different from those used in calibration. It is important to have data from a wide range of forcing functions (measurable attributes) that are defined by the objectives of the model (RG_{S_1}). Validation criteria (RG_{S_2}) are formulated on basis of the objectives of model (RG_{S_1}) and the quality of the data.

2b) Suppose that a slight variation in the data of one of the measurable attributes takes place. In such case we should move from $\Psi_{ij} \Rightarrow \Psi'_{ij}$ where Ψ'_{ij} is synonymous of Ψ_{ij} . Therefore, it would go from A_j to A'_j , that is to say, from the sentence A to its synonymous sentence A'. The synonymous will be found in the orbitals but what is more important is that this movement is erratic defining a brownian or Wiener process. With this criterium the state equations will be stochastic differential equations (SDE).

3. Finally we show a third process of recognoscibility, denoted by RG_{S_3} . This process is based on those words generated by the recognoscitive grammar RG_{F_2} . For each state equation, defined in terms of sentences, a coefficient of determination d_k , defined from the corresponding coefficients of determination r_{ij}^k of the flow equations which form the sentence, may be defined

$$d_k = \frac{\sum_{j=1}^{1_k} r_{ij}^k}{1_k}, 0 \leq d_k \leq 1$$

where 1_k is the length of the sentence or number of flow equations that constitutes it. We define d_k as a **complex determination coefficient of the state equation**.

When a state equation has a coefficient of determination d_k , it is transformed into a stochastic differential equation and we could speak about stochastic state equations (SSE).

2.7. Dissipation Function and Flow Orbital

We assume constant the conjugate force to the flow process. This, as stated, may be represented by a determined flow equation or by flow equations orbital. In

the latter case, Prigogine's equation becomes the following:

$$\sigma^*_i = \{\Psi_i(X)\}^* \cdot \Delta_i(X); i=1,\dots,n \quad (27)$$

Therefore, for a given system H, flow processes can be represented as being σ_i^* the dissipation orbital function of flow process P_{Ψ_i} , having the orbital n synonymous equations. Therefore, for a given system H, flow processes can be represented as

$$\sigma_{\Psi} = \sum_j \{\Psi_i(X)\}_j^* \cdot (\Delta_i(X))_j; \quad (28)$$

$$i=1,\dots,n; j=1,\dots,m$$

Such expression given the dissipation function of m flow orbitals of system H, corresponding to m flow processes.

3. Conclusions and Perspectives

From the above we can draw the following conclusions:

1. Each imbalance produces a force, each force causes a flow process, each flow is represented by a flow variable that is formally written as an equation, known as flow equation, and if each flow tends to equilibrate the system, the equations mathematically represent the tendency to balance.

2. The same flow process has a number of flow equations that represent it. These equations have each other, a relationship of synonymy, forming an equivalence class.

3. There is a subset of synonymous equations, which define the same flow process, within which are the synonymous equations with highest fit, that is, with higher occurrence probability. This subset has been called flow orbital.

4. It is possible to obtain the function of dissipation of a given flow equation, of a flow orbital and of flows process system.

Dissipation function is a measure of the entropy produced by the system. Dissipation functions of flow equations present the following questions:

1. To what extent is there a relationship between the dissipation functions obtained by the theorem of Prigogine and deduced through the flow functions?.

2. What is the relationship between entropy determined by these functions of dissipation and linguistic entropy obtained in Text Theory of ecological models developed by the authors (Sastre-Vazquez et al., 1999, 2000; Usó-Domènech et al., 1997^b, 1999^{a,b}, 2000, 2001, 2002, 2006^{a,b}; Villacampa et al., 1999^{a,b}; Villacampa and Usó-Domènech, 1999^{a,b})?.

Only a deepening of the theoretical studies and a strong experimentation with real data can clarify the answers to these questions.

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