A Model Based on Chemical Reaction for the Neural Processes Involved in Cognition*

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Abstract
After briefly reviewing current psychological and neurophysiological knowledge about cognitive processes it is presented a chemical reaction paradigm which allows quantitative analysis of their dynamics. It is also made a reinterpretation of the model in terms of dendro-dendritic local computations as well as of somato-axonal communication at a distance. It is suggested the possible utility of this model for the understanding of psychopharmacological therapy of mental disorders.
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1 Psychological, Psychophysiological and Neurochemical Dimensions of Cognitive Processes. Some Anatomical Requirements for The Integration of Functional Processes.

An adequate hypothesis about the correlates of cognitive processes poses many requirements beyond the admission of a distributed parallel computation in the brain. The episthemic diversity of the experimental sources of the data gathered along distinct lines of investigation in different functional components in the Encephalon renders necessary the use of a multi-level structural model- which takes into account new computational paradigms together with new proposals about the neural embodiment of psychological dimensions. Some concepts, concerning learning theory allow the

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characterisation of classical and instrumental conditioning, in the context of connectionist mechanisms embodied in neural nets.

Tolman's views are relevant historical examples of an attempt to avoid the rigidity of models of conditioned reflexes through the introduction of the concepts of an inner space of representation of internal and external events and the admission that expectancies (anticipations), perceptions, emotions, values are needed to represent the interaction between an organism and its environment. Such an approach implies the use of symbols to represent concepts and sensory, motor, emotional, motivational patterns.

Semantic access and memory, work memory, decision making processes, intentional behaviour and predictive processes suggest a constructivist model in which encoding processes establish a functional implementation of distributed high level computations. This model implies bottom-up and top-down matches between symbolic rules and connectionist networks.

The role of Hippocampus in the consolidation of long term memory records in a parallel distributed manner, together with local specific data, is a relevant paradigm. Hyperincursive computation in sequences of intentional behaviour is a main component of anticipatory processes which as a matter of fact imply the use of processes which are part of an inner representation of events which occur in the external environment as well as in the internal environment. A main characteristic is the association of these processes and internal time and space coordinates for the process of decision making and planning of actions and the use of external time and space coordinates for the process of execution of real interactions. Sensory information is supposed to be used when it attains the final stages at the highest level of pattern identification of data in a bottom-up computation.

Abstract conceptual information matches the representation of immediately acquired sensory data by means of top-down processes which add representations of patterns of action, as well as foreseen results and predictions of emotional reactions and valences that orient data acquisition.

Decision making processes are directed by executive, orienting and vigilance attention which superintend the performance of acts, and the acquisition of information during the performance of intentional strategies.

Alternative plans are subjected to a choice that depends on a definition of goals and subgoals which are concatenated under a motivational reference framework and an abstract meta-representational control.

It is at this level of abstract conceptual command and control that we find the ensemble of regularities on which we may base the understanding of an executing Self.

On the other hand at the level of computational processes we propose a paradigm obtained in Quantum valence and orbital theories that is used to produce an insight about possible ways for neuronal encoding of interneuronal binding connections through characteristic periodic oscillation frequencies.

Periodic signals in dendro-dendritic networks encode the local binding between neuronal operative structures. The activation of these characteristic oscillations is set through axonal transmission at a distance.

Quantum valence theory provides a model for both the strength of the binding connections and on the other hand the superimposition of the frequencies that encode functional and labeling messages.

If we consider as a paradigm the link of two hydrogen atoms A and B in a single molecule through a covalent bond in orbital s in both atoms, combining the possibilities of formation of the bond by each one of the two electrons in each atom, as well as the shielding effect exerted by non-bonding electrons, we obtain

$$\psi = \psi A(1)\psi B(2) + \psi A(2)\psi B(1) + \lambda\ \psi A(1)\psi A(2) + \lambda\ \psi B(1)\psi B(2)$$

where ψ is the characteristic wave function of the bond.
More complex molecular structures would require the consideration of Resonance phenomena. This paradigm may be useful to provide a work hypothesis concerning interneuronal binding through a functional and dynamic process.

The binding of the distinct representational and executive units which perform concurrent computations would depend on labels encoded in the frequency domain. These labels would carry information about the abstract conceptual framework which directs the organisation of adaptive processes and simultaneously would perform a programming action.

They would play a role in the self-organisation of local connectionist structures which are assembled to form new operational units. In a neurophysiological approach available evidence indicates that executive schemes as well as informational maps are also distributed over sub-cortical structures belonging to the Basal Ganglia as well as to the Thalamus, Hypothalamus, Cerebellum and Reticular System, and on the Associative Cortex of the Brain.

This way representational, motivational and valorative dimensions of information are distributed with local distinctive characteristics that qualify a specific functional viewpoint which potentially may contribute to the global cognitive representation.
From a psychological viewpoint the relevant role of the conscious dimension implied by the cognitive self-reflexive characteristics of such processes would result first from an 'eigen time-space procedural structure' in which distinct decision processes are

embedded. Future goals, present data, past situations would be coordinated by this procedural scheme which embodies the construction of a dynamic representation of an action, under the form of a set of local decision rules and data. This representation would be associated to an intention as far as the possible role of perceptive data and actions is involved.

Even pure perceptive knowledge architectures would embody the latent possibility of exerting an intention which would imply an exploratory information gathering and goal fulfilling strategy.

The conscious quality of experience would require the internal construction of a referential procedural structure which simultaneously carries recursive and hyperincursive computations.

The conceptual structure which would provide the references necessary to evaluate the efficiency of a representation and an action would correspond to an intervention, from a psychological viewpoint of a structure that would be called the Self. In our model it would result from the regularities of the action of orienting, executive and vigilant attention, together with a preferential choice of motivational orientations and characteristic affective reactions.

Again, from a neurophysiological viewpoint, the binding function of attention would be supported by both Parietal Lobes, Anterior Cingulate Regions, Supplementar Motor Areas, the Reticular Formation of the Mesencephalon, the Associative Nuclei of Thalamus, both Frontal Lobes and the Right Cerebellar Hemisphere.

For a cognitive model of an interaction it is furthermore necessary the consideration of a complementary representation which includes, beyond the characteristic actions over the environment, the dynamics of the action of the environment over the organism.

2 The Chemical Reaction Paradigm

Let us suppose a poorly feedforward linear neural network with inputs $\bar{X}$ and outputs $\bar{Y}$ which receives sensory information from a mosaic of visual receptors and performs Principal Components Factor Analysis and identifies straight line segments with different orientations in space.

We further admit that the output $\bar{Y}$ interact with a solution of multiple chemical reactors A, B, ..., Z.

$\bar{Y}$ components react in parallel with one or more of the reactors available in the solution. The rate of this reaction will be different for components K, L, M. These different rates will depend on some energy parameter T and on the distinct concentrations of reactors K, L, M, ..., respectively.

With all conditions kept constant the final equilibrium state will depend on the temperature, the concentrations and the characteristic rates of reaction under the energising parameter T.

Interpreting each reactor as an operator which assembles the outputs $y \in \overline{Y}$, we have described an equivalent for a process in which components $y \in \overline{Y}$ are linked to reactors to form new Ky, Ly, ... The dynamics of the reaction will ensure a ranking of the final concentrations. If those components were the inputs for some coordinated patterns of action, the ranking in concentrations would produce a selection favouring the execution of actions according with the difference in concentrations.

Let us suppose a feedback information for these actions which acts as a 'critic' changing of some parameters- for instance the energising factor T which could be interpreted in a neurophysiological perspective as an action due to Reticular System of the Brainstem and of the Thalamus. This change in T would differentially affect the rate of the distinct reactions and the final equilibrium state.

Furthermore an input $\overline{I}$ for the chemical solution would differentially increase the concentration of the different reactors according with the critical evaluation of the actions being performed.

Interpreting this feedback in neurophysiological terms would lead us to consider it as a result of an interaction with the Limbic System which commands and controls affects.

The change in the T and concentration parameters might be accompanied by a change in the volume of the solution thereby producing the possibility of formation of new and complex reactors- for instance AB, AC, ..., ABC, ABD, ..., ACD, ..., ABCD, ... These new compounds would be equivalent to more complex neurophysiological operators which would perform pattern constructions which would again compete for the elicitation of decisions of action- this would be equivalent to a Work Memory included in an Executive Attention and Vigilance process.

3 Some Chemical Characteristics of the Process

If we consider parallel chemical processes we must distinguish the stirred tank model which is not described by differential equations because there are no spatial changes nor changes in time. The case of spatial changes corresponds to the batch reactor and time changes will be considered in the context of Plug Flow Reactor (PFR).

3.1 Batch Reactors

Within the batch reactor metaphor, processes in a dendro-dendritic complex provoke the formation of 'compound messages' such that the time needed to attain a 'steady state' for a new compound message Ay is

$$t = -\frac{1}{k}\ln\frac{N_{Ay}}{N_{Ay0}} \tag{1}$$

In (1) N_{Ay} stands for the number of messages of a class at any instant, and N_{Ay0} that number at t=0. k is related to the 'reaction rate', something like the readiness of the dendro-dendritic net to produce new messages.

Now, a main feature of the batch reactor analogy is the potentiality to generate parallel processes, besides the serial ones, which lead to some kind of anastomatic computation. For parallel 'reactions' the proportion of different compound messages can be written as

$$S = \frac{\alpha_{Ay\cdot A}}{\alpha_{Ay\cdot A} + \alpha_{By\cdot A}} \tag{2}$$

where $\alpha_{Ay.A}$ is the proportion of compound Ay and $\alpha_{By.A}$ is the proportion of By. In any case these parameters are introduced to illustrate the potentiality of the metaphor.

In case the 'compound message' triggers the adequate patterns of action, the Ascending Reticular System of the Brain Stem and of the Thalamus will energise the rate of production of that 'compound message' performing an action equivalent to a reactors' temperature elevation during an adequate time interval Δt_i. The following classical reactor equations express the idea that 'compound message formation' rate will effectively increase with a raise of temperature, in a reversible endothermic reaction. At equilibrium, $r_A=0$; $x_A=x_A^*$ (x_A^* is the reactant conversion at equilibrium) and substituting into the reaction rate expression we have,

$$\frac{x_A^*}{1-x_A^*} = \frac{k_1}{k_{-1}} = K = \frac{k_1'}{k_{-1}'}\exp\left(\frac{\Delta E_{-1} - \Delta E_1}{RT}\right) \tag{3}$$

In (3) ΔE_1 is the forward activation energy which must be greater than the reverse activation energy, ΔE_{-1}, k_1 and k_{-1} are defined by

$$r_A = k_1 C_A - k_{-1} C_B \tag{4}$$

In (4) C_A is the concentration of A and C_B is the concentration of B.

In case the 'compound messages' are no longer adequate, the energising action of the Reticular System ceases, and a new ensemble of sets of characteristic dendro-dentric oscillators will be activated, renewing the cycle of interactions which will now include new dendro-dendritic operators. Not that it is implied that reactants change but not the form of the reactions.

Finally, Work Memory and Executive Attention will activate new areas of the Brain and associate Sub-Cortical structures which will create a similar but distinctly organised functional architecture, until the Intentional action is completed. What changes here in the model is the type of relationships between isolated reactions which become organised in a structured system. To embody Work Memory and Executive Attention Control and Command, a dendro-dendritic network of fully connected multiple centres in the sense that any centre is connected by inputs and outputs to all the remaining ones and to itself, forms a sort of a 'keyboard' that is able to be activated sequentially or in parallel and in turn produce changes in the pattern of relationships between more elementary units that are organised by the 'keyboard'. A switching control makes a temporal plan of activations according with a prescribed set of criteria which act within the context of local time relationships which form an invariant pattern for decision making. This local time and space parameters form the context necessary for an internal model representation of an interaction with the environment (Tolman, 32, 38) using both recursive and hyperincursive goal directed computations which generate behaviours which will be performed according with external time-space parameters and produces a state which represents the interaction from the viewpoint of internal decision making performed according with local time-space parameters completely distinct from the external ones. In our hypothesis the set of decision making rules, the 'keyboard' programming of both plans of action and connected internal representations, internal local time-space relationships and the availability to an self reflexive knowledge about this processes in a summarised manner in which many links are missing, forms the basis for conscious awareness of the environment, of the Self, and of both elementary decisions and complex plans of action and Intentions.

Central planning of action furthermore recruit, at a distance, other specialised operators to produce new processes made from a different viewpoint. These centres which work in a distributed manner make decisions of action and back propagate information about their actual state of activity. They correspond to Tertiary Multisensory Associative Areas, as well as to centres responsible for the use of linguistic competence and idiomotor symbolic representations of commands of structured action.

These high level centres either non linguistic or else linguistic will send encoded messages, that upon being received, play a role in the programming of the commands and representations to which they are contributing. Possibly it is the encoded structure of this high level symbolic messages that performs the double role of carrying a semantic content and simultaneously specific programming of relational instructions.

In order to obtain a chemical reaction model for this structure we would, in first place, consider the Quantum approach towards valence either Ionic valence or Covalent valence. Considering the characteristic orbitals of elements, we would be able to specify 'compound messages' with a high degree of complexity.

We consider these complex 'compound messages' as being produced in multimodal sensory processes, Cognitive processes or else, hybrid combinations of sensory motivational, emotional, cognitive, volitional, linguistic and ideo-motor plans of action.

We will not enter in the details of these aspects here. We will rather consider the possible 'reactions' between them along a time of processing considering, as a first approach to a model, the example of Plug Flow Reactors (PFRs) (Levenspiel, 72; Metcalfe, 97).

4 Neuronal Implementation - The Dendro-Dendritic Network Model

If we consider neural architectures, dendro-dendritic networks possess the remarkable characteristic of allowing both forward and backward propagation. The complex geometry of these networks permits back propagation of action potentials generated at the axon hillock. Ultimately when such potentials attain fine dendritic ramifications they can eventually fade out. When this is not the case such potentials can circulate along dendro-dendritic closed loops which implement local computations.

Although dendro-dendritic networks are extremely dense anatomical structures with interspersed almost reticulate structures linked by multiple synapses, they may be thought of as an ensemble of computational compartments. Let us consider the case in which information arrives to the dendritic neuropile through axo-dendritic and dendro-dendritic synapses.

If we attribute to each neuronal cell body a set of characteristic dendro-dendritic closed loops we may consider each such set as an ensemble of oscillators with characteristic frequencies. We assume that complex information processing is performed by each neuron due to its closed loops. Similar functions are served by identical sets of closed loops and distinct functions are implemented by different sets of closed loops, A, B,..., Z.

If the same information arises to an ensemble of distinct sets of closed loops each one performing the analysis and processing of the incoming information from a distinct viewpoint, we may assert that an input vector {Y} (coming from the output of a predecessor structure) activates distinct sets A, B, ..., Z of dendro-dendritic closed loop operators.

From the viewpoint of our analysis it may be considered that 'compounds' Ay, By, ..., Zy have been formed and the corresponding information will be transmitted by neuronal cell bodies at a distance to decision making neurons responsible for the generation of coordinated patterns of action. A, B, ..., Z, are closed loop operators and oscillators $y \in \{Y\}$ are a subset of ordered components of $\{Y\}$ with dimension $\dim.(y) \leq \dim(\{Y\})$.

This interaction will be comparable to the formation of a new 'compound' Ky which triggers patterns of action when it reacts with receptors E forming a new 'compound' KyE.

In the case of a batch reactor the time needed to attain the steady state of the formation of a new 'compound message' Ay is given by

$$t = -\frac{1}{k}\ln\frac{N_{Ay}}{N_{Ay0}} \tag{5}$$

In (5) N_{Ay} stands for the number of moles of Ay at time t in volume V (the system), N_{Ay0} stands for the initial number (at t=0) of Ay in the same volume V, k is defined by

$$r_{Ay} = k\,C_{Ay} \tag{6}$$

In (6) r_{Ay} is the reaction rate and C_{Ay} is the concentration of Ay. In our case in which we considered parallel reactions the proportion of different 'compound messages' will be given by

$$S_{Ay.A} = \frac{\alpha_{Ay.A}}{\beta_{Ay.A}} = \frac{\alpha_{Ay.A}}{\alpha_{Ay.A} + \alpha_{By.A}} \tag{7}$$

In (7) $\alpha_{Ay.A}$ is the conversion of product Ay, β_A is the conversion of reactant A and $\alpha_{By.A}$ is the conversion of product By and $S_{Ay.A}$ is the overall selectivity for the product Ay.

The quantity of the second 'compound message' By will be given by an identical equation with conversion coefficient α_{By}. The instantaneous or local selectivity, $\phi_{Ay.A}$, is based upon the instantaneous or local reaction rates,

$$\phi_{Ay/A} = \frac{r_{A1}}{r_A} = \frac{r_{A1}}{r_{A1} + r_{A2}} \qquad (8)$$

In (8) r_{A1} is the reaction rate of the reaction A→Ay and r_{A2} is the reaction rate of the reaction A→By.

A similar equation gives the value of $\phi_{By.A}$.

In case the 'compound message' triggers the adequate patterns of action, the Ascending Reticular System of the Brain Stem and of the Thalamus will energise the rate of production of that 'compound message' performing an action equivalent to temperature elevation during an adequate time interval Δt_i. The following equations show that 'compound message formation' rate will effectively increase with a raise of temperature, in a reversible endothermic reaction. At equilibrium, $r_A=0$; $x_A=x_A^{*}$ (x_A^{*} is the reactant conversion at equilibrium) and substituting into the reaction rate expression we have,

$$\frac{x_A^*}{1-x_A^*} = \frac{k_1}{k_{-1}} = K = \frac{k_1^{'}}{k_{-1}^{'}}\exp\left(\frac{\Delta E_{-1} - \Delta E_1}{RT}\right) \qquad (9)$$

In (9) ΔE_1 is the forward activation energy which must be greater than the reverse activation energy, ΔE_{-1}, k_1 and k_{-1} are defined by

$$r_A = k_1\, C_A - k_{-1}\, C_B \qquad (10)$$

In (10) C_A is the concentration of A and C_B is the concentration of B.

In case the 'compound messages' are no longer adequate, the energising action of the Reticular System ceases, and a new ensemble of sets of characteristic dendro-dentric oscillators will be activated, renewing the cycle of interactions which will now include new dendro-dendritic operators. Not that it is implied that reactants change but not the form of the reactions.

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5 Concluding Remarks

The main feature of this model is the identification, in this context, of orbitals of elements and periodic oscillations with characteristic frequencies in dendro-dendritic closed loops for each neuron.

Quantum Valence Theory and the characteristic orbitals will impose restrictions in the types of 'compound messages' that may be found.

The model of chemical reactors was used to provide reference structure for cognitive processes within a specific theoretical framework.

In this context the analysis of reaction rates provides a tool for studying convergence conditions from a quantitative viewpoint very distinct from the usual qualitative cognitive models. Furthermore the use of models of catalytic reactions will allow the integration of neurotransmiter actions in cognitive operations and hopefully provide an explanatory system for the understanding the action of psychotropic drugs used in psychopharmacological interventions.

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