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MATLAB in Biomodeling

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1. Introduction

Mathematical modeling and computer simulations are widespread instruments used for biological systems study.
Matlab and Simulink are powerful, high-level programming language which offer the opportunity to apply the principles of linear systems theory in the analysis of biological systems; the opportunity to develop adequate computer simulation techniques and algorithms in order to model dynamic responses of physiological systems, and to collect and analyze data and to visualize the results information for the simulation processes

2. Systemic modeling in biosciences

Models are extremely useful in understanding how the neuronal cell stores, computes, integrates and transmit the information necessary for the survival of the organism. Computer assisted models permit also to create a variety of test scenarios that would be too difficult, expensive or dangerous to allow to happen in reality.
The main goal in modeling and simulation in the area of Biosciences is to develop integrative models and simulation which allow the dynamic representation of signaling and metabolic networks in the neuronal cell as open systems with distinct input and output ports and specific response mechanisms. The systemic approach in the actual researches in the field of biomodeling aim to fit together the different level at which complex biological systems are working, from genes through cells, organs to the whole organism (Noble, 2002). The majority of biological and physiological control systems are nonlinear and the control is often accomplished parametrically.
Biological systems are hierarchical systems, characterized by:

1. Each level has unique language, concepts or principles;
2. Each level is an integration of items from a lower level; discoveries or descriptions at i^{-th} tlevel aid understanding of phenomena at i+1 level;
3. Relationship between levels is not symmetrical;

In fig.1. is presented the algorithm used for developing biological systemic and mathematical models. Control systems theory, applied in the neuronal modeling, is used to analyze the dynamic properties of the neuronal metabolic and signaling pathways and to understand the role of feedback loops in the reaction networks. The essence of this approach lies in the dynamics of the system and cannot be described merely by enumerating the components of the system. In the systemic approach, the neuronal cell is considered an open system with distinct input and output ports and specific response mechanisms.

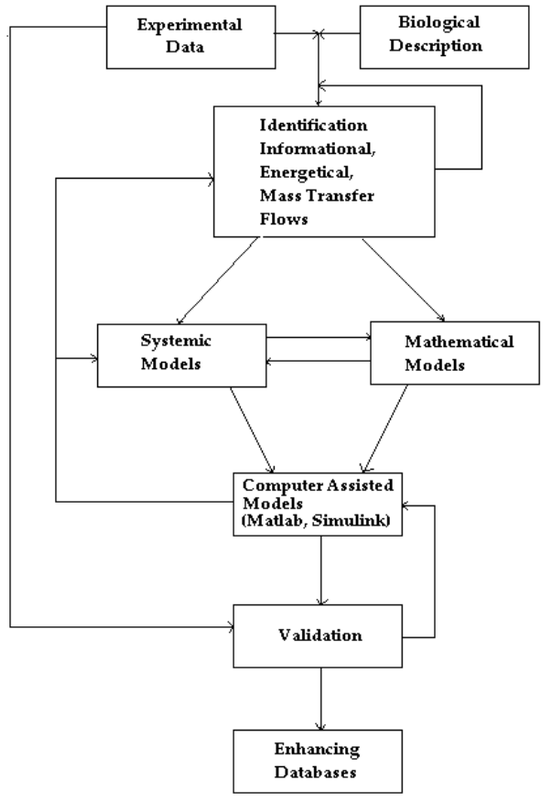

Fig. 1. The algorithm for developing systemic and mathematical models in neurobiology

Biological systems are adaptive systems, stable, equipped with control mechanisms (feedback) extremely fine (Heinrich, 1996). In fig.2 we have considered a model rule to regulate processes within the neuron, a model that, in various forms, otherwise we will find all subprocesses in regulating cell.

In the neuronal cell, extracellular and intracellular stimuli are captured and measured by specialized receptor structures located in the cytoplasm and in the cell membrane. Stimuli are represented by various substances that circulate in the body (hormones, oxygen ions, different protein structures), environmental factors (radiation, temperature variations, etc.) and electrical impulses from adjacent cells. Based on these stimuli, and coded programs to DNA, control mechanisms (feedback) provides nerve cell adaptation to environmental conditions. They aim to develop cell responses to stimuli coming from the external environment and internal, depending on the deviation e(t) measured between the model output (encoded at the genetic level) $y_M(t)$ and output biosystem (neuronal cell) y(t).

$$\varepsilon(t) = y_M(t) - y(t) \tag{1.1}$$

Under ideal operating conditions for the neuronal cell $\varepsilon(t) \to 0$

Where:

u(t) = input size

r(t) = size reference

y(t) = output size

p(t) = disturbance

Models about the mechanisms of neuron refers to adaptive changes in cell metabolism, compared with the extracellular environment. In the presence of enzymes, synthesized as a result of chemical reactions, substances taken from the cell improper turns feeding their cell substance. Exchange with the outside is permanent and will work antientropic cell, because it will prevent their growth through disruption of entropy.

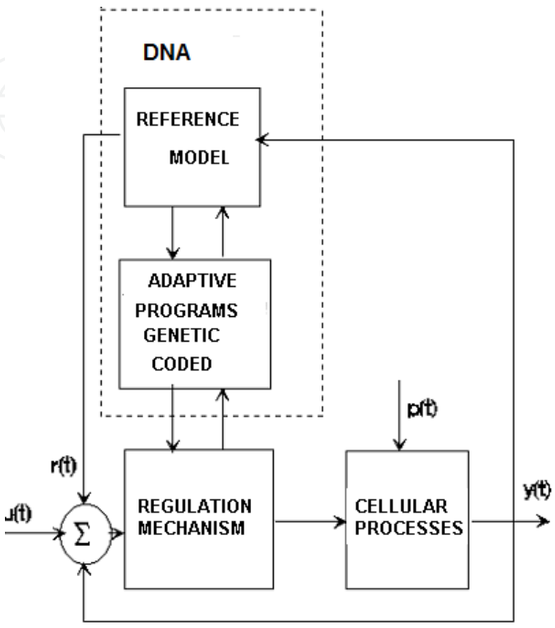

Fig. 2. The systemic model for the regulation processes in the neuronal cell

3. Neuronal cell processes modeling

3.1 The systemic and mathematical models of protein synthesis in the neuronal cell

From the systems theory viewpoint, the neuronal cell is an open system with distinct input and output ports and specific response mechanisms. Signaling action through the pathways result in different categories of cellular responses like ionic channel opening or closing, neuronal differentiation or neuronal cell death. The dynamical models of signaling pathways are nonlinear and the analysis of their behavior in challenging request specific algorithms.
In a first approximation, the protein synthesis process at neuronal level may be modeled like a open three-compartmental system (fig.3.)

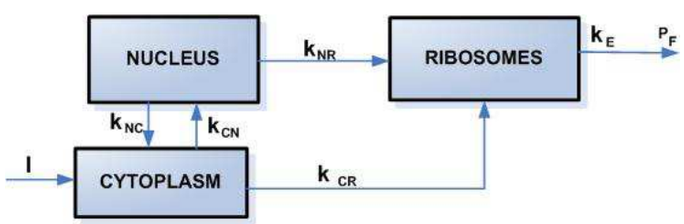

Fig. 3. The three-compartmental model for the protein synthesis process

The equilibrium equations which are describing the system are:

$$\frac{d}{dt}q_N(t) = (-k_{NC} + k_{CN})q_C - k_{NR}q_R \tag{2.1.1}$$

$$\frac{d}{dt}q_C(t) = (k_{NC} - k_{CN})q_N - k_{CR}q_R + i(t) \tag{2.1.2}$$

$$\frac{d}{dt}q_R(t) = k_{NR}q_N - k_{CR}q_C - k_eP_f(t) \tag{2.1.3}$$

Passing in the matrix form, we have:

$$\frac{d\bar{q}}{dt} = A\bar{q} \tag{2.1.8}$$

$$\begin{pmatrix} q_N(t) \\ q_C(t) \\ q_R(t) \end{pmatrix} = \bar{q} \qquad \frac{d}{dt}\begin{pmatrix} q_N(t) \\ q_C(t) \\ q_R(t) \end{pmatrix} = \frac{d\bar{q}}{dt} \qquad \begin{pmatrix} 0 \\ I(t) \\ -k_eP_f(t) \end{pmatrix} = \bar{b} \tag{2.1.5}$$

$$\begin{pmatrix} 0 & (-k_{NC} + k_{CN}) & -k_{NR} \\ -(-k_{NC} + k_{CN}) & 0 & -k_{CR} \\ k_{NR} & k_{CR} & 0 \end{pmatrix} = A \tag{2.1.6}$$

Using the substitutions (2.5) and (2.6) we get the next afine equation:

$$\frac{d\bar{q}}{dt} = A\bar{q} + \bar{b} \tag{2.1.7}$$

With the initial condition: $\bar{q}(t_0) = \overline{q_0}$

In order to solving this equation, we have firste to determinate the solution of the homogenous equation:

$$\frac{d\bar{q}}{dt} = A\bar{q} \tag{2.1.8}$$

The General solution of such an equation is:

$$\bar{q}(t) = Ce^{A(t-t_0)}, A \in M_{3,3}(R) \tag{2.1.9}$$

where:

$$e^{A(t-t_0)} = \sum_{n\geq 0} \frac{A^n(t - t_0)}{n!} \tag{2.1.10}$$

The proper values of matrix A, used in the study of the protein synthesis process stability are:

$$\begin{aligned} \lambda_1 &= 0 \\ \lambda_2 &= i\sqrt{k_{CR}^2 + k_{CN}^2 + k_{NR}^2} \\ \lambda_3 &= i\sqrt{k_{CR}^2 + k_{CN}^2 + k_{NR}^2} \end{aligned} \tag{2.1.11}$$

The main biochemical process in the protein synthesis is the formation of the peptide bound. The necessary information for the synthesis of a protein is stored at the specific structural gene level coded as purines and pyrimidine bases of DNA molecule structure. To each amino acid is corresponding a characteristic group of three bases, called codon, the total number of specific combinations being 64. Through a process of transcription, the code is transferred in the form of an m_{RNA} molecule, synthesized in the nucleus and then transferred into the cytoplasm. The RNA molecule acts on the ribosomes, in the initiation stage of synthesis process. During the transcription process, each sequence of DNA is copied into a corresponding sequence on the m_{RNA}.

The RNA synthesized in the neuronal cell nucleus is transferred through the nuclear pores in the cytoplasm in two forms: m_{RNA} and t_{RNA}, each of the two macromolecular structures fulfilling specific roles in the synthesis the proteins. Also, in the cytoplasm of amino acid activation occurs in the presence of ATP, under the influence of specific amino-synthase, resulting in an amino-AMP synthetase complex. In this specific t_{RNA}, also synthesized by the DNA transcription synthase is released, forming amino acid-activated t_{RNA} complex.

Amino acids activated and coupled with t_{RNA}, reach the ribosomes structures where protein synthesis takes place in three phases:

- initiation phase
- elongation phase
- termination phase

In the protein synthesis process are implied:

- DNA
- Amino acids
- Ribosomal RNA (r_{RNA})
- Messenger RNA, formed the nucleus (m_{RNA})
- Cytoplasmic transfer RNA (t_{RNA})
- Enzyme activation of amino acids (amino t_{RNA}-synthase)
- Initiation Factors
- Transfer Factors
- Termination factors

The initiation phase

The protein synthesis process is triggered under the influence of initiation factors existing in the cytoplasm, and, especially, the m_{RNA}, which contains an initiation codon Uracil-Guanine-Adenine (UGA), which is fixed on the 40S ribosomal subunit. On the initiation codon is fixing the initiation t_{RNA}, which is containing the initiation anticodons (sequence complementary codon UGA) and carries the emtionina. The t_{RNA} initiation is carried at the P-site P-peptidyl from the 60S subunit (Haulica, 1997).

The elongation phase

On the codone that follows the initaiting one, is fixing itself the corresponding t_{RNA} which is bringing the first aminoacid from the proteic sequence, and positioning itself on an second site (A) from the 60S subunit. When two t_{RNA} molecules are fixed on the ribosome, is acting a ribosomal transpeptidase which is transferring the formilmetioninic residue from the P site t_{RNA} on the A site t_{RNA}, forming a dipeptidil-t_{RNA} is. Then, through a phenomenon of translocation, during which the ribosome dipeptidil-t_{RNA} is and moving in opposite directions on the distance of a codon, dipeptidil reach the site of P-t_{RNA}, and the site of, remained open, it's loaded with fixed t_{RNA} the second amino acid sequence. By repeating the process, to add new amino acids, in accordance with the code sent. The process described is carried out based on energy supplied by ATP and GTP, and elongation of existing factors in the cytoplasm (Haulica, 1997).

The terminal phase

Is triggered by m_{RNA} termination codon (UGA or UAA), reached the site of the codon A. t_{RNA} is not fixed, but protein termination. At this point, unlink transpeptidase peptide chain composed of the last t_{RNA}. Peptide passes into the cytoplasm, being separated into ribosomal subunits (Haulica, 1997).

Based on bio-physiological processes described above, we have developed the following model for the systemic process of protein synthesis in the neuronal cell (fig.4), where:

DNA = deoxyribonucleic acid

m_{RNA} = messenger ribonucleic acid

t_{RNA} = transfer ribonucleic acid

r_{RNA} = ribosomal ribonucleic acid

In the cytoplasm, the conservation equations for t_{RNA} and m_{RNA} mass will be:

$$\frac{dM_{RNA_t}}{dt} = Q_{RNA_{t_P}} + Q_{RNA_{t_L}} - Q_{RNA_{t_D}} - Q_{RNA_{tAMP}} \tag{2.1.12}$$

$$\frac{dM_{RNA_m}}{dt} = Q_{RNA_{m_P}} + Q_{RNA_{m_L}} - Q_{RNA_{m_D}} - Q_{RNA_{m_R}} \tag{2.1.13}$$

Where:

M_{RNAm}, M_{RNAt} = mass of m_{RNA}, respectively mass of t_{RNA};

Q_{RNAmP}, Q_{RNAtP} = m_{RNA} flows, respectively t_{RNA} flows, coming from the nucleus into the cytoplasm through nuclear pores;

Q_{RNAmL}, Q_{RNAtL} = m_{RNA} flows, and that t_{RNA}, which are in free state in the cytoplasm;

Q_{RNAmD}, Q_{RNAtD} = m_{RNA} flows, and that t_{RNA}, degraded citosolic nuclease;

Q_{RNAmR} = flow mRNA, ribosomal binding sites linked in t_{RNA};

$Q_{RNAtAMP}$ = = flow, which combined with amino-AMP-synthetase complex, forming a complex amino acid-activated tRNA (Dabu, 2001)

When the cell is in rest, we have:

$$\frac{dM_{RNA_m}}{dt} = 0 \tag{2.1.14}$$

$$0 = Q_{RNA_{m_P}} + Q_{RNA_{m_L}} - Q_{RNA_{m_D}} - Q_{RNA_{m_R}} \tag{2.1.15}$$

$$\frac{dM_{RNA_t}}{dt} = 0 \tag{2.1.16}$$

$$0 = Q_{RNA_{t_P}} + Q_{RNA_{t_L}} - Q_{RNA_{t_D}} - Q_{ARN_{tAMP}} \tag{2.1.17}$$

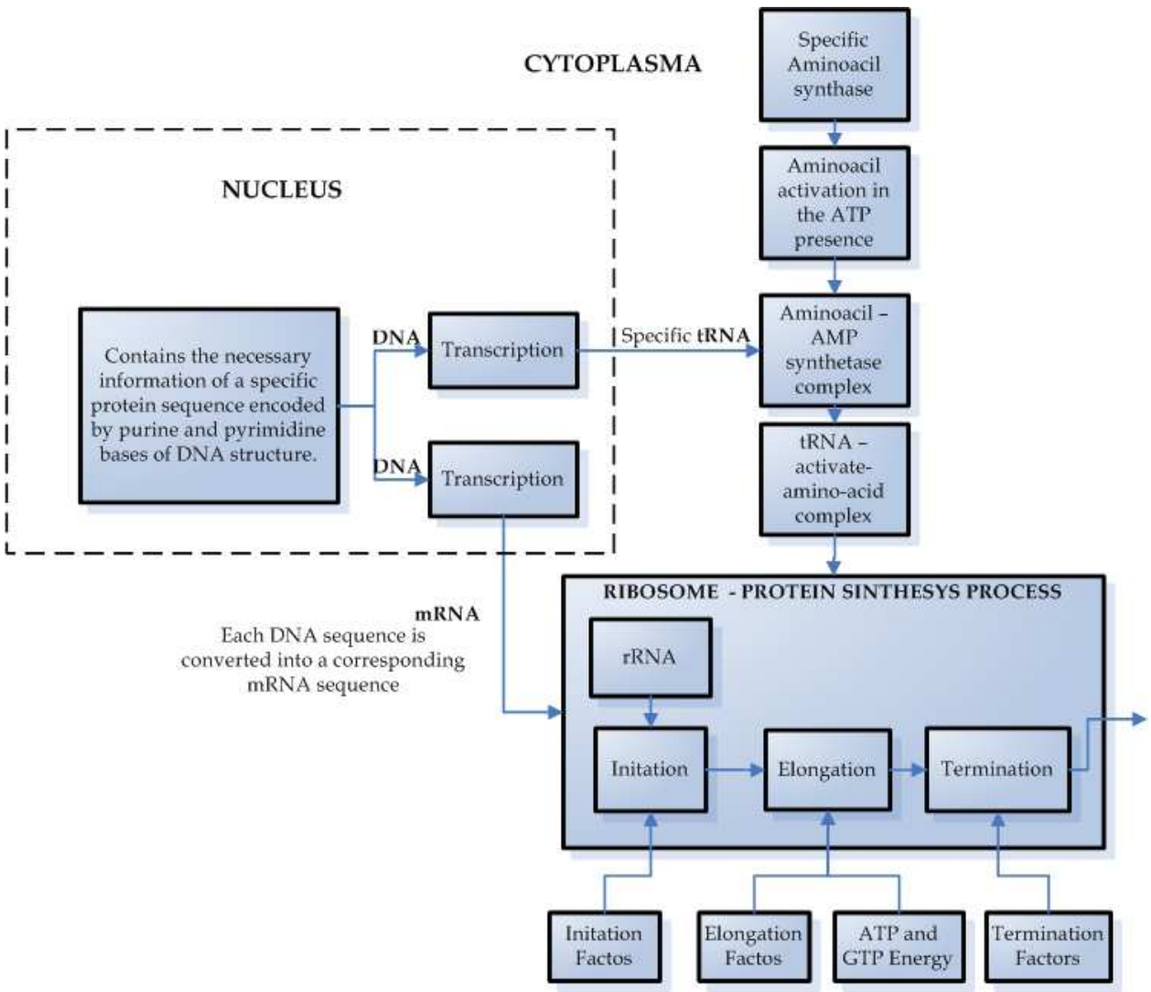

Fig. 4. The multi-compartmental model of protein synthesis process in the neuronal cell

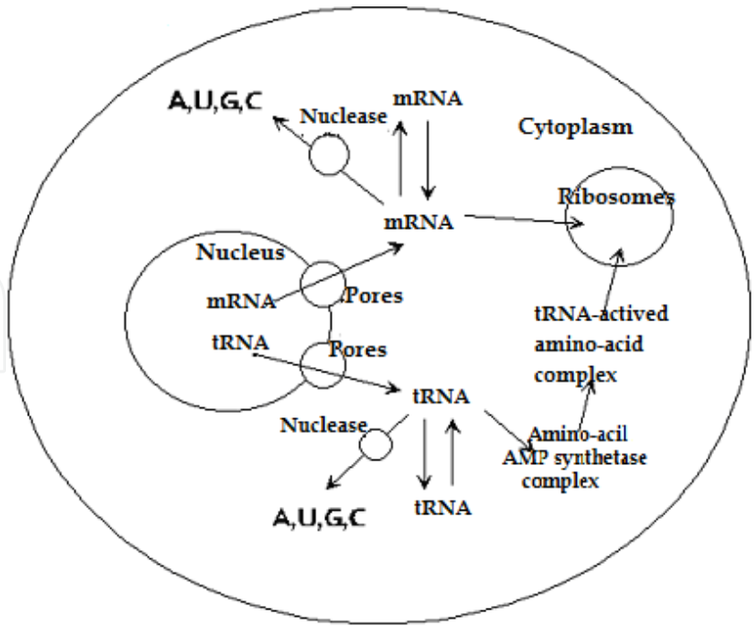

Fig. 5. Chart status for tRNA and mRNA in the neuronal cell

3.2 Modeling the behavior of Ca^{2+} ions as second messengers

The dynamical model for the Ca^{2+} regulation is nonlinear and the analysis of this process behavior request specific algorithms and tools. MatLab and Simulink offer adequate tools and algorithms for modeling these kind of processes.

In a neuronal cell in resting state, Ca^{2+} concentration is maintained at values below 10^{-7} mol/l, because the existing balance between influx and efflux of Ca^{2+}. Ca^{2+} influxes that may come from outside the cell by IL-type channels, the ISA, the messengers I, or G protein receptor complex or other messengers (cAMP, cGMP, IP4). Another source is the influx of Ca^{2+} stores in cell Ca^{2+} bound in the mitochondria or reticulum endo (sarco) plasma. Increasing concentrations of free cytoplasmic Ca^{2+} is compensated (in the idle state of the cell) by effluxes equivalent achievement either to exter (pump ATPase Ca^{2+} receptor-operated and how other messengers II system and antiport third Na^{+}/Ca^{2+}) or to deposits (by the Ca^{2+} ATPase) (Haulica 1997).

Cell activation through the occurrence of an action potential (AP) or through the coupling action of a messenger I with specific receptors, stimulates the Ca^{2+} influx and mobilization of deposits. When the concentration of cytoplasmic free Ca^{2+} exceeds the threshold value of 10^{-5} mol/l, cell response is triggered by Ca^{2+} as second messenger. Depending on the receptors involved in the process and the path followed, cell responses may get different aspects: the degradation of cAMP and cGMP, the formation of cGMP and cAMP, glycogenolysis, the release of synaptic neuromediators, protein synthesis, etc.

The effects of activation of other second messengers, Ca^{2+}-CaM complex, modulatory activated creates the possibility of two or more lines of receptor-activated intracellular signaling a significant effect on the final pool of the cell response (Rousset et al. 2003)

3.2.1 Modeling the behavior of neuronal Ca^{2+} when cell is in rest

When the cell is at rest, free cytoplasmic Ca^{2+} concentration is maintained at values below 10^{-7} mol/l, and the system is described by the following equation (Dabu, 2001):

$$\begin{cases} \dfrac{d[Ca_L^{2+}]}{dt} = Q_{Ca^{2+}I_L} + Q_{Ca^{2+}I_{SA}} + Q_{Ca^{2+}Msg_I} + Q_{Ca^{2+}G} + Q_{Ca^{2+}Mit} + Q_{Ca^{2+}RE} - \\ \qquad\qquad -Q_{Ca^{2+}EATP} - Q_{Ca^{2+}LATP} \end{cases} \quad (2.2.1)$$

Where:
$[Ca^{2+}_L]$ = concentration of free Ca^{2+} in nerve cell cytoplasm in a state of rest;
$Q_{Ca^{2+}IL}$ = influx of extracellular Ca^{2+} ion channels IL;
$Q_{Ca^{2+}ISA}$ = influx of extracellular free Ca^{2+} ion channels ISA;
$Q_{Ca^{2+}\ MsgI}$ = free extracellular Ca^{2+} influx through messengers I.
$Q_{Ca^{2+}G}$ = free extracellular Ca^{2+} influx through G protein;
$Q_{Ca^{2+}Mit}$ = flow freely from the mitochondrial Ca^{2+} deposits
$Q_{Ca^{2+}RE}$ = free flow of Ca^{2+} from the endoplasmic reticulum;
$Q_{Ca^{2+}EATP}$ = efflux by intracellular free Ca^{2+} ATPase pump;
$Q_{Ca^{2+}LATP}$ = intracellular free Ca^{2+} flux through the ATPase of caught and stored Ca^{2+} in mitochondria

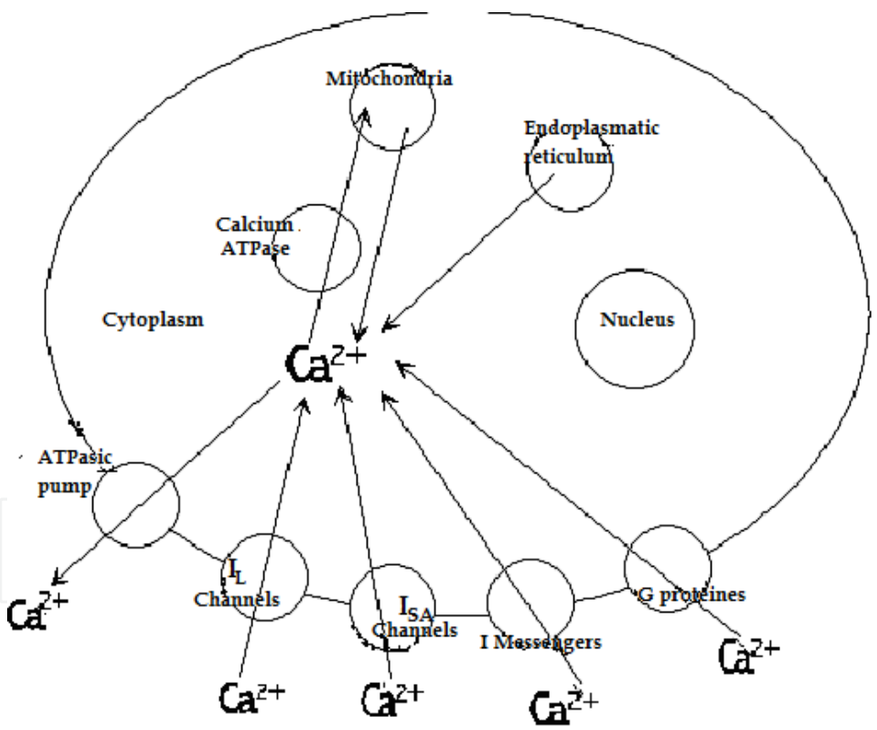

Fig. 6. The states chart for Ca^{2+} inside the neuronal cell in rest state

3.2.2 The cellular response modeling

Ca^{2+} acts as a messenger II in activating the cellular response when the neuronal cell is activated either by the occurrence of an action potentialor after coupling a messenger I with a specific receptor and the concentration of Ca^{2+} free in the cytoplasm exceeds the threshold

value of about 10^{-5} mol/l. At the occurrence of an action potential in the neuronal cell as result of releasing the synaptic mediator in the synaptic space, the membrane depolarization at terminal button level stopes the penetration of Na^+ from outside the cell and generate the increasing of Ca^{2+} influx inside the cell.

The ions penetrate from the extracellular environment through two kinds of channels:

1. voltage-dependent Na^+ channels opened by action potential
2. voltage-dependent ionic channels, which are opened with a certain delay.

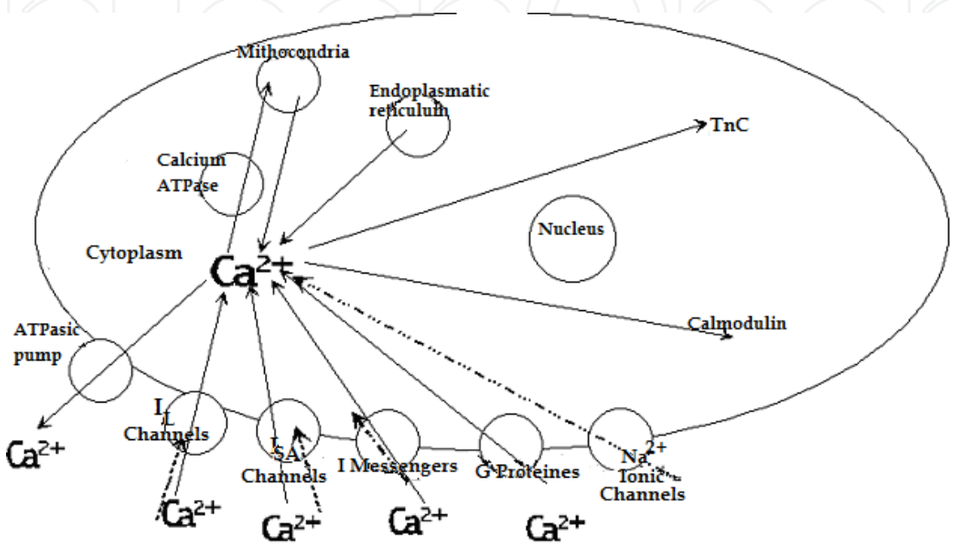

Fig. 7. States diagram for the free Ca^{2+} as cell reponse initiator in the activated neuronal cell cytoplasm

$$\begin{cases} \dfrac{d[Ca_L^{2+}]}{dt} = Q_{Ca^{2+}I_L} + Q_{Ca^{2+}I_{SA}} + Q_{Ca^{2+}Msg_I} + Q_{Ca^{2+}G} + Q_{Ca^{2+}Mit} + Q_{Ca^{2+}RE} + \\ \quad + Q_{Ca^{2+}Na^+} - Q_{Ca^{2+}EATP} - Q_{Ca^{2+}LATP} - Q_{Ca^{2+}Cmd} - Q_{Ca^{2+}TnC} \\ \dfrac{d[Ca_L^{2+}}{dt} \geq 0,99 * 10^{-5} \end{cases} \quad (2.2.2)$$

Where:

$[Ca^{2+}_L]$ = free concentration of the nerve cell cytoplasm in rest state;

$Q_{Ca^{2+}IL}$ = influx of extracellular Ca^{2+} ion channels IL;

$Q_{Ca^{2+}ISA}$ = influx of extracellular free Ca^{2+} ion channels ISA;

$Q_{Ca^{2+}MsgI}$ = free extracellular Ca^{2+} influx through Messengers I channels.

$Q_{Ca^{2+}G}$ = free extracellular Ca^{2+} influx through G protein channels;

$Q_{Ca^{2+}Mit}$ = flow freely from the mitochondrial Ca^{2+} deposits

$Q_{Ca^{2+}RE}$ = free flow of Ca^{2+} from the endoplasmic reticulum;

$Q_{Ca^{2+}EATP}$ = efflux by intracellular free Ca^{2+} ATPase pump;

$Q_{Ca^{2+}LATP}$ = intracellular free Ca^{2+} flux through the Ca^{2+} ATPase of captured and stored in mitochondria Ca^{2+};

$Q_{Ca^{2+}Na^+}$ = Ca^{2+} influx through voltage-dependent Na^+ channels opened by action potential

$Q_{Ca^{2+}Cmd}$ = free flow of cytoplasmic Ca^{2+} which combines with Calmodulin

$Q_{Ca^{2+}TnC}$ = free flow of cytoplasmic Ca^{2+}, which combine with TnC
In order to developing the model in SIMULINK, in order to describe the behavior of intracellular Ca^{2+} as messenger II, the following things were considered:
- description of the biological process
- analysis of a great number of lab tests regarding the behavior of Ca^{2+} , including:

The models that were built are characterized by the fact that, for input data that is similar (from the point of view of equivalence with the real world) to measurable input data for the real system in laboratory conditions, the output data, from point of view of values and evolution in time, was very close to the experimental data obtained from the lab tests.
Also, the obtained models have been verified, to establish their validity and adjustments were made where it was required, for a higher fidelity of the models.
The models were developed with MATLAB 4.2 for Windows and SIMULINK 1.3. In their development, the following were considered:

1. Intracellular Ca^{2+} is one of the most important messengers II, having a decisive role in secretion, motility, intermediary metabolism, cellular division, and cell death;
2. Intracellular Ca^{2+} concentration is very important in information processing at neuronal level;
3. The mechanisms for regulation of Ca^{2+} distribution within a neuronal cell include mainly non-linear processes, whose kinetics depends both on time and space
4. Not all the sub-systems that contribute to the regulation of intracellular Ca^{2+} concentration operate at the same rate. Some are rapid systems, while others are slow systems, with delays and idle periods;
5. Research demonstrated the existence of more Ca^{2+} transport sub-systems at neuronal level: mitochondrial sub-system, endo(sarco)plasmatic reticulum sub-system, ionic channels transportation, Ca^{2+} ATPases transportation and transport through Na^{+}/Ca^{2+} ion exchangers
6. Laboratory tests carried out on mouse hippocampus cells demonstrated that, following and action potential, intracellular Ca^{2+} concentration could reach the value of 1mM, while, at rest, intracellular Ca^{2+} concentration is about 0.1 mM. Laboratory tests analysis, performed with the FURA-2 system have shown that the induction of an intracellular depolarization, following 10-20 action potentials, increases the level of intracellular Ca^{2+} concentration within soma and proximal apical dendrites from 0.02-0.05 mM to 0.1-0.2 mM. The time required for the concentration level to come back to the initial value was about 100 ns. Other similar Laboratory tests analyzes have shown that the level of intracellular Ca^{2+} concentration could increase by 400-500% as a response to an electric pulse applied for 500 ms, with a comeback to the initial value period of 5 s.
7. Fluctuation of the Ca^{2+} concentration at cell level depends on:
   - the volume of the substance where the process takes place;
   - local diffusion coefficient
   - geometry of the elements and structures analyzed (Dabu,2008)

In figures 8 and 11 are presented the Simulink models for the regulation of the Ca^{2+} in the neuronal cell in rest state and activated state of the cell. The input ports are the input ionic channels and receptor sites from the neuronal membrane where signaling molecules initiate coupled sets of chemical reactions within the cellular space The output ports are the output ionic channels and the specific binding sites from the neuronal membrane where the signaling molecules are binding and initiate bio-chemical reactions outside the cell.

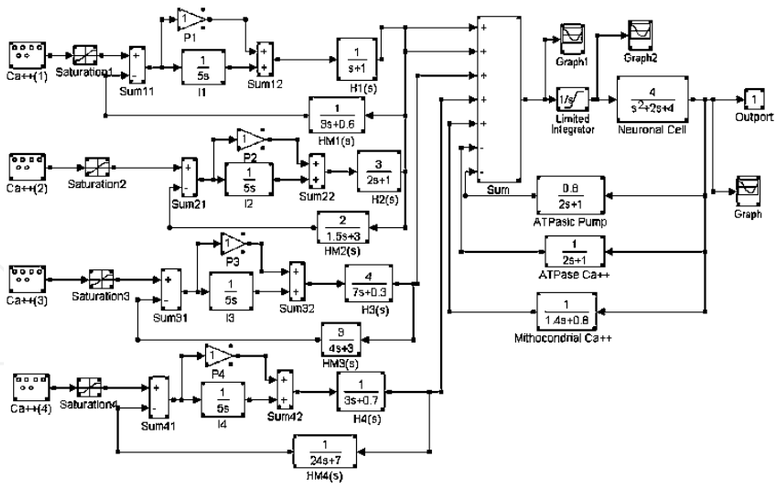

Fig. 8. The Simulink model for the regulation of the Ca^{2+} in the rest state of the neuronal cell

The results of the simulations are Presented in figures 9 and 10

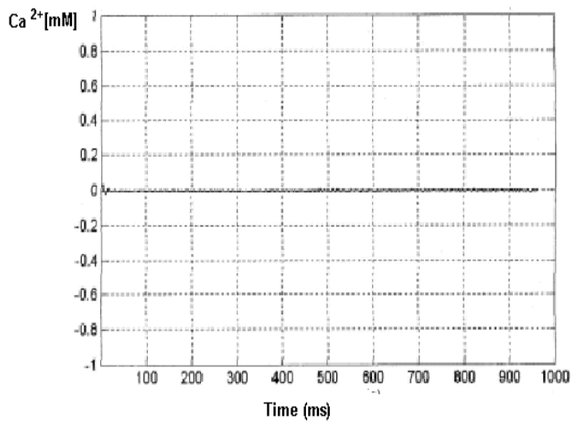

Fig. 9. Simulation results with low variation of Ca^{2+} concentration

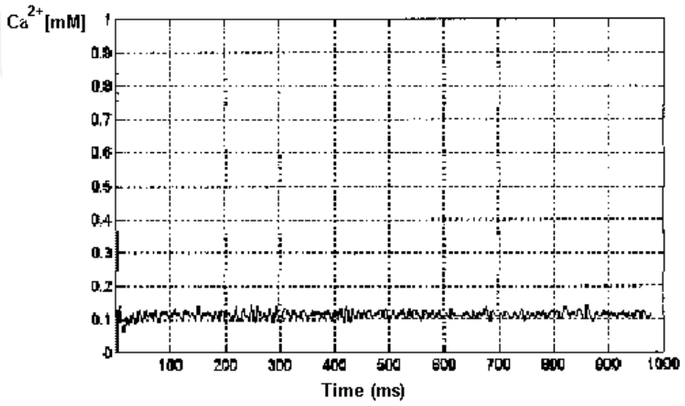

Fig. 10. Simulation results with higher variation of Ca^{2+} concentration

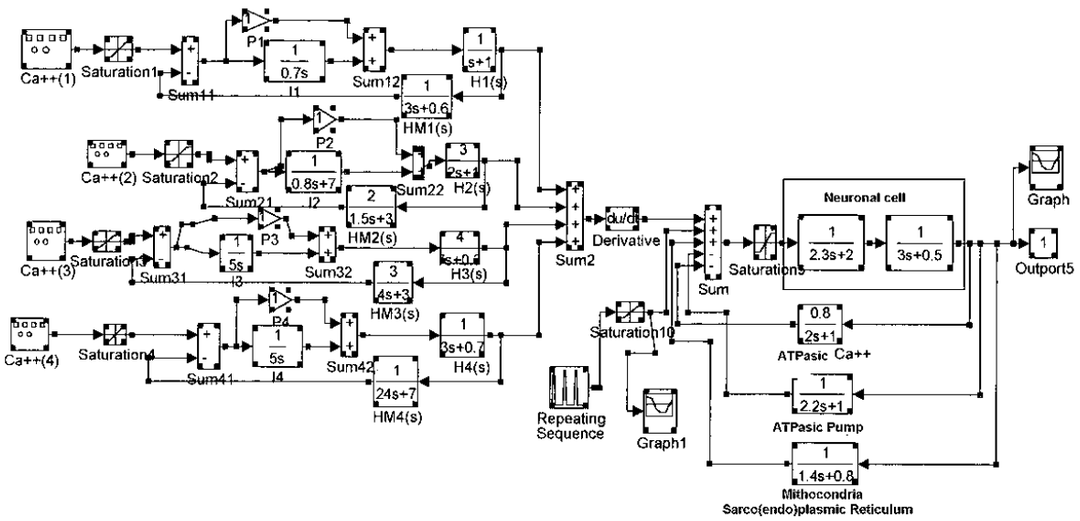

Fig. 11.The Simulink model for the regulation of the Ca^{2+} in the activate state of the cell

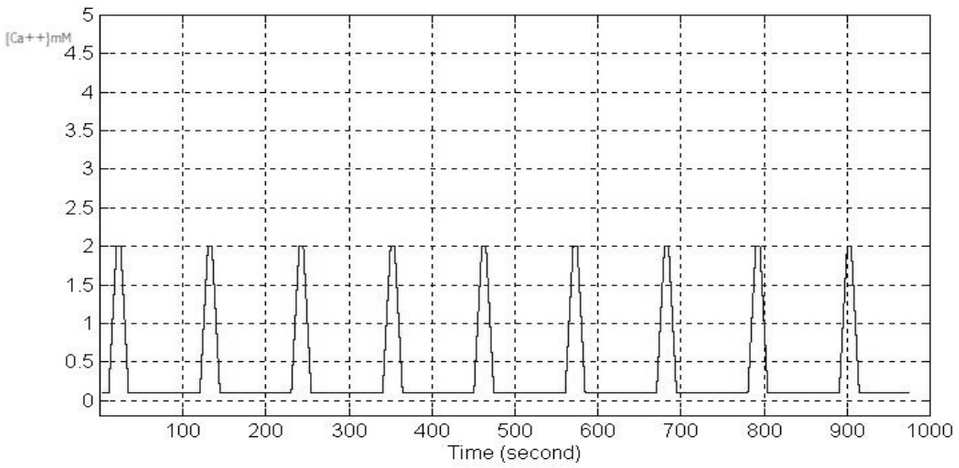

Fig. 12. Simulation for the activate neuronal cell

4. Matlab and simulink in computer assisted modeling and systemic approach for aerobic bioremediation

The aerobic bioremediation treatment process technology use special bacteria blends engineered in order to biodegrade the organic contamination (fig. 13) into harmless carbon dioxide and water, to derive energy, with no potential environmental impacts, as compared to conventional burning methods. Some of the carbon is used by bacteria as ”food” to derive new carbohydrates, proteins and nucleic acids for growth. One bacteria category is initializing the process, and other bacteria families are continuing the process (figure 2). The absence of one bacteria species from the bacteria blend is diminishing the purifying capacity of the whole system .

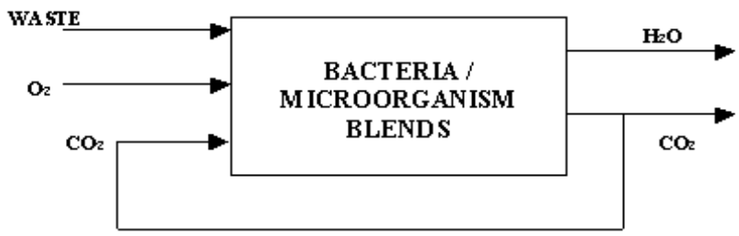

Fig. 13. The systemic model for aerobic bioremediation

For bioremediation to be effective, microorganisms must enzymatically attack the pollutants and convert them to harmless products. As bioremediation can be effective only where environmental conditions permit microbial growth and activity, its application often involves the manipulation of environmental parameters to allow microbial growth and degradation to proceed at a faster rate. The most used procedures for environmental parameters manipulation are: biosparging, bioventing, the use of oxygen releasing compounds; pure oxygen injection, hydrogen peroxide infiltration, ozone injection. All these procedure add in the contaminated area supplemental supply of oxygen which becomes available to aerobic, hydrocarbon-degrading bacteria. Like other technologies, bioremediation has its limitations. Some contaminants, such as chlorinated organic or high aromatic hydrocarbons, are resistant to microbial attack. They are degraded either slowly or not at all, hence it is not easy to predict the rates of clean-up for a bioremediation exercise. There are no rules to predict if a contaminant can be degraded (Rockne et al., 2000).

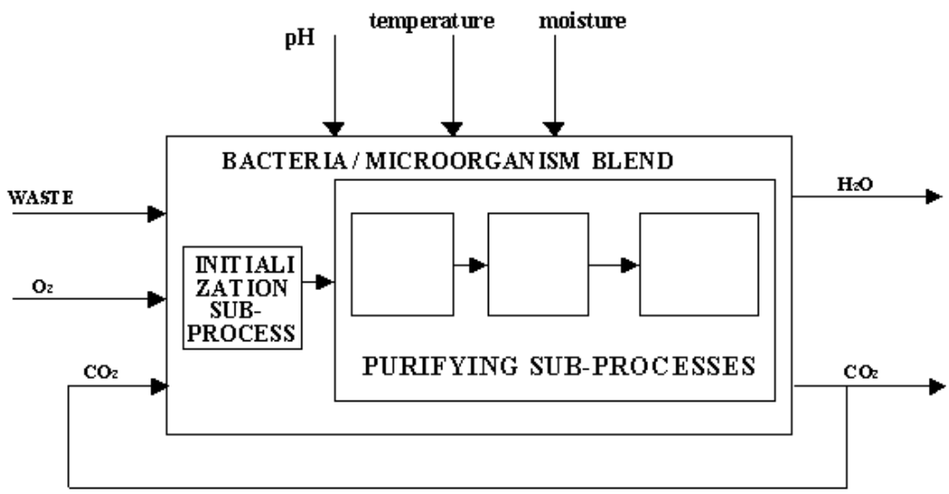

Fig. 14. The compartmental systemic model for aerobic bioremediation

Microbial growth and activity are readily affected by pH, temperature, and moisture. Temperature affects biochemical reactions rates, and the rates of many of them double for each 10°C rise in temperature. Above a certain temperature, however, the cells die. Available water is essential for all the living organisms, and irrigation is needed to achieve the optimal moisture level. The amount of available oxygen will determine whether the system is aerobic or anaerobic (fig.14)

Biomodeling using Simulink and Matlab can provide important answers regarding the mechanisms of biodegradation reactions and the evolution of degenerative capabilities in bacteria/microorganisms. They are usefully to predict the outcome of the bioprocesses and to evaluate the time and the costs of the intervention, it is necessary to create and use systemic and computer assisted mathematical models to describe the bioremediation processes (Dabu 2004).

For developing such models, it is necessary to look down the following steps:

1. Establishing the scope of the required treatment;
2. Identifying the inputs and outputs of the system;
3. Identifying the environmental parameters which affect the process and the corresponding sub-processes (bioavailability, penetration or uptake of the compounds trough the cell envelope, flow and transport, biochemical reactions, release of products);
4. Identifying the inhibitory and activator effects of different compounds or microorganism classes;
5. Identifying the compartmental systemic model of the process.
6. Identifying the transfer functions which are describing every compartment of the model and the transfer function for the entire model (Dabu & Nicu 1998, Dabu 2004).

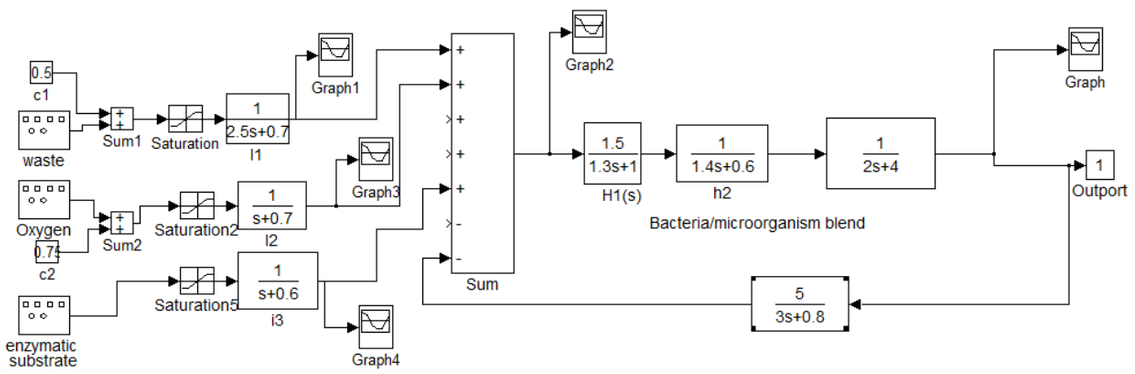

Fig. 15. The Simulink model for an anaerobic bioremediation process

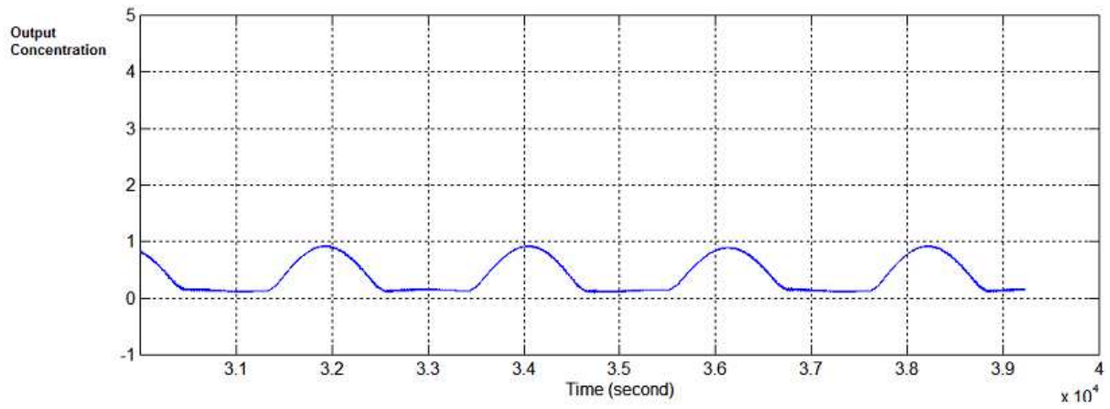

Fig. 16. The simulation output

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MATLAB - A Ubiquitous Tool for the Practical Engineer

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A well-known statement says that the PID controller is the â€œbread and butterâ€ of the control engineer. This is indeed true, from a scientific standpoint. However, nowadays, in the era of computer science, when the paper and pencil have been replaced by the keyboard and the display of computers, one may equally say that MATLAB is the â€œbreadâ€ in the above statement. MATLAB has became a de facto tool for the modern system engineer. This book is written for both engineering students, as well as for practicing engineers. The wide range of applications in which MATLAB is the working framework, shows that it is a powerful, comprehensive and easy-to-use environment for performing technical computations. The book includes various excellent applications in which MATLAB is employed: from pure algebraic computations to data acquisition in real-life experiments, from control strategies to image processing algorithms, from graphical user interface design for educational purposes to Simulink embedded systems.

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