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CYBER-PHYSICAL SYSTEMS IN ELECTROCHEMICAL MEASUREMENTS

Annotation. Effectiveness of cyber-physical systems in electrochemical measurements was analyzed. It was shown that measurements connected tightly environment, computation and communication; the whole system is multi-dynamic, with feedback interaction between 'cyber' and 'physical' parts; volume of data to be processed is unlimited in many cases. These features of the process are typical for cyber-physical systems' application domain.
Key words: cyber-physical system, electrochemistry, simulation, measurement.

1. Introduction. The term 'cyber-physical systems' (CPS) refers to integration of computation with physical processes [1]. Usually, the term used to describe embedded systems as well as networks monitoring and controlling physical processes which, through feedback circuits, can affect computation flows. They combine cyber capabilities (communication, computation and control) with physical capabilities (sensing and actuation) to solve problems that neither part could solve alone. Physical processes are compositions of many parallel processes. Hence, CPS are intrinsically concurrent. CPS are multi-dynamical ones: mathematical models laying in their foundations are compositions of multiple elementary dynamical aspects. CPS produce computer control decisions and are, thus, discrete. At the same time they are continuous, because they are based on differential equations of motion or other physical processes. CPS are uncertain, because their behavior is subject to choices coming from environmental variability or intentional uncertainties that simplify their model. This uncertainty can manifest in different ways [2]. Uncertainties make CPS stochastic when good information about the distribution of choices is available. Uncertainties make CPS nondeterministic when no commitment about the resolution of choices is made. Uncertainties make CPS adversarial when they involve multiple agents with potentially conflicting goals or even active competition.

Huge potential of cyber-physical approach to design of modern computer systems is indicated by its fast expansion into new domains of application. Now they include health care, transportation, process control, large-scale infrastructure, defense systems, tele-physical operations and others. Such approach seems to be very effective in solving problems arising in the field of electrochemical measurements as well.

2. The problem. There exists a vast variety of methods and devices to obtain data about electrochemical processes under investigation. The size of the paper leaves no chance to consider all of them, so optical, gravimetric, isotopic techniques were set aside for further analysis; our attention will be focused on voltammetry of electrochemical objects. Electrical characteristics to be measured may relate both to potentials and to currents occurring in the object.

Typical CPS may support following functions:

- potential/current programming control;
- sensor preparation/renovation;
- thermal control;
- hydrodynamic control;
- reagents input;
- data collection and processing;
- decision making;
- self-testing.

Analysis of requirements to corresponding subsystems of a CPS is given below.

2.1 Potential/current programming control. According to Le Chatelier principle, an electrochemical object tries to eliminate all outer effects by changing its state, potentials of its constituents in particular. Usually these potentials are measured against special reference electrode [3]. If currents are under control, electronic circuits based on operational amplifiers are used. Sometimes, e.g. in impedance spectroscopy, stationary potential is controlled while alternative current is changed according with independent

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time schedule. Such schedule can be previously elaborated by experimenter in very general terms and often must be corrected during the measurement. In the case of CPS these corrections assume selection of new object's mathematical model and sometimes changes in time scale of characteristics' control as well as of computation process.

In relaxation techniques one often expects linear response of the electrochemical object on outer perturbation; this linearization can be realized by applying further restrictions on potential/current program control, that, in turn, depends on preliminary selection of the object's model; the model may be changed during the experiment, too. Thus, one can see requirements to the computer system such as necessity of multi-scale dynamical control of the environment with mutual influence object's state and computational process, specific for CPS. Models used in the subsystem's computation can be both discrete and continuous.

2.2 Sensor preparation/renovation. In many versions of electrochemical measurements the working electrode must be brought to and kept in certain state during the measurement (the surface activity, electrode's size and/or shape). In the case of liquid electrode (mercury and melted metals) it forms growing drop; so, the measurement must start at certain moment of its growth. When transitional processes run rather quickly, jet of electrolyte may be used as conducting medium between electrodes. In this case initial moment of perturbation must be synchronized with start of electric connection (jet's arrival). Again, dynamics of liquid within the jet is crucial for proper organization of computing and communication in 'cyber' part of CPS.

Working electrode often has to be activated because of passivated film on its surface. There are different ways to perform this procedure. The simplest one is mechanical renovation (dripping, cutting/grinding *in situ*). It requires proper synchronization of the renovation ending with measurement's start. More complicated technique demands application of serial galvanic pulses to the electrode. Number, duration, frequency and amplitude in the pulse series may be determined in previous experiments empirically or be calculated according to given mathematical model; interaction with such feedback loops between 'cyber' and 'physical' is typical for CPS.

2.3 Internal mode control. Thermal control is rather simple task; usually it should not go beyond the object thermostatting and can be solved by use of corresponding electronic devices. For large industrial objects like plating bath simulation of temperature distribution is of great importance; corresponding models are based on systems of differential equations.

Models applied for hydrodynamic mode control vary from very simple to rather sophisticated when the object under consideration includes airlift, rotating electrodes, porous media and so on. Fortunately, feedback from environment to controlling subsystem is not crucial in the case of regular measurements under stationary hydrodynamic modes.

Simulation of reagents' concentrations can not be supported by modern embedded processors in real time mode; the problem is even more complicated because the species can react with each other, settle out or leave the object through exhaust ventilation. That is why this subsystem primarily serves for weight filling and blending reagents within the object. Locations of dosers must be determined during the system design.

Self-testing subsystem is obligatory if one needs to obtain reliable data. Drift of analog-digital converters, heating of inner parts of 'cyber' system, need in periodic calibration of actuators, sensor failures make it necessary to use expert subsystems for estimation of measurement reliability.

2.4 Data processing and decisions making. In previous sections it was shown that the process of the electrochemical measurement produces various data flows of different nature and importance, in different time scales and very often (e.g., at corrosion monitoring) of infinite volume. Data processing requires simulation in real time with application of broad scope of mathematical models; in many cases these models may be switched during the measurement. Dynamics of the environment effects on computation and demands dynamic reorganization within 'cyber' part of the system. Neural nets and other intellectual blocks are regular parts of the decision subsystem. (For example, state of corroding construction needs for adequate estimation 27 parameters to be taken into account).

3. Results. Brief analysis given above shows that even speaking about voltammetry only one can obtain reliable data and make adequate decisions

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when cyber-physical system is at work. Measurements connected tightly environment, computation and communication; the whole system is multi-dynamic, with feedback interaction between 'cyber' and 'physical' parts; volume of data to be processed is unlimited in many cases.

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Кіберфізичні системи в електрохімічних вимірюваннях

Проведено аналіз ефективности застосування кіберфізичних систем в електрохімічних вимірюваннях. Показано тісний зв'язок між оточенням, обчислювателем та комунікаційною системою в процесі вимірювання; система як ціле мультидинамічна, "кібернетична" та "фізична" частини завдяки зворотнім зв'язкам взаємодіють між собою; об'єм інформації що обробляється в багатьох випадках нічим необмежений. Такі властивості процеса характерні в областях застосування кіберфізичних систем.

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