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NETWORK FOR EPR SPECTROSCOPIC ANALYSIS AS A TOOL IN DIDACTIC PROCESS

The paper deals with a new training technologies' development based on distance learning web-services, implemented for laboratory of a Pharmacy Study branch at Medical University in Katowice. The discussed computing interfaces allow students to perform analysis of free radicals' spectra provided by EPR device. These training facilities are now available at home; at their remote terminal. The training resources consist of electronic / computer based training. The laboratory provide the students with an interface incorporated into simulation packages along with statistic apparatus for data analysis. The dynamically configured application provide the user with his individual set of training samples. Additionally it provides a valuable skill training for students, otherwise available only as part of master of science thesis work.

1. INTRODUCTION

The laboratory experiments usually require very expensive equipment that should be incorporated effectively, for every student separately, into its training process. The pharmaceutics and the medical diagnosis branches are no exception. These very demanding and complex issues depend on training interfaces given to an individual user.

The laboratory classes, guided by a teacher, are a common practice in the majority of schools. Students, in most cases, suffer from the shortage of time to recognise fundamentals – especially vital in case of the pharmacy study. They also need reminding of any details while doing projects or diploma works.

In our everyday work with students, many limitations are noticed. The student needs an access into the laboratory, in an unpredictable moment, often when the University labs are already closed. On the other hand the devices are too expensive to be provided for every student individually during laboratory classes.

The computer and e-learning technologies, with networking (Internet) facilities, provide us with interesting abilities of multiplying the number of users working on a virtual machine, using experimental data.

The paper presents the solution incorporated in the pharmacy department. The multiple access into one device using several remote analysis tools was introduced. A second section describes several technical issues, while developing the proposed tool. The third section shows the implementation details along with medical device integration issues as well as experiment feedback from users. Finally, the further works within this area, were also discussed.

2. THE SOLUTION'S ENVIRONMENT AND ASSUMPTIONS

The easiest way for a more effective training organisation goes through the laboratory equipment size; with many work stations available at any time, for every student. There are many reasons, one can find, that this idea cannot be considered as a proper solution. The most important ones are tremendous costs and large space of the laboratory.

The remote access into the laboratory equipment became available thanks to the wide area of computer network services. This virtual laboratory idea needs a specific, dedicated equipment and

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software packages, fulfilling these expectations. The remote training methods are found very encouraging [1,7,8,9], not only because of remarkable reduction of the equipment costs but also by easy and comfortable access into the laboratory units.

The experiments on the laboratory station are usually enriched with simulation packages [2,3]. The simulation packages are guiding the user through the application, with many comments for understanding the analysis details (to reach the mastery, as a final goal).

The proposed laboratory organisation was introduced in Fig. 1. It consists of three main parts: e-learning system, proposed tool (along with sample database) and the laboratory device itself. To simplify the implementation and migration of solution, the tool can be added to any LMS platform as a part of a course. The presented work was tested in Moodle.

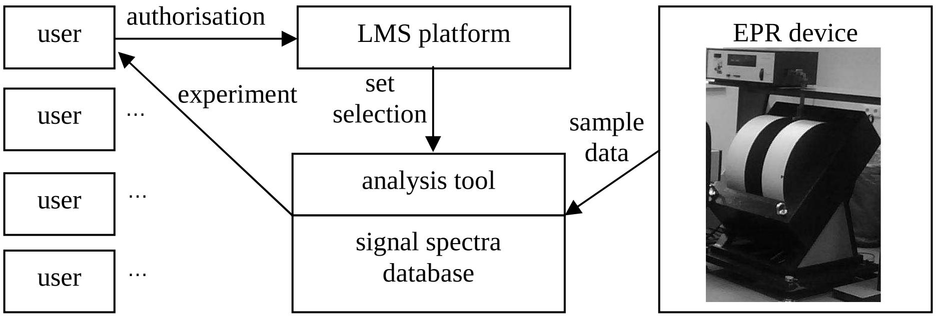

Fig. 1. The laboratory services organisation.

The laboratory network works under the control of a main machine (running 24 hours a day), where the presented tool, with its software units is installed. The platform provides the application with communication with e-content, performing the users' knowledge evaluation.

The communication interface for virtual laboratory is powered by the Flash technology that is supporting the Learning Management Systems (LMS) as well e.g. MOODLE - the more and more popular platform recently. These units are supported by reach libraries and services, as:

- XML document engine[10] for manifests processing,
- evaluation mechanisms ([4,5]) for real time user interaction measurements.

The EPR laboratory device, which generates data for analysis, is a vital part of the presented method. In this method we use database obtained as the EPR spectra recorded by Rapid Scan Unit of Jagmar Firm (Kraków). The EPR device is isolated from a network, for security reasons. The system collects new samples' data on request. Only the spectra database process can communicate with the data acquisition process in EPR device. The network denies access from other devices and services [6].

3. TOOL IMPLEMENTATION

Program useful to spectroscopic analysis of the first derivative EPR spectra was constructed. Electron paramagnetic resonance spectroscopy (EPR) is the experimental method applied to determination of properties of paramagnetic systems [12-14]. Paramagnetic are the samples containing free radicals with spin S = 1/2, biradicals with spin S = 1, paramagnetic ions, π electrons delocalized on multi-ring aromatic units [12-14]. Paramagnetic properties reveal also oxygen molecules O2 in the ground state with spin S =1 [12]. Paramagnetic centers with unpaired electrons are the very important species in medicine and pharmacy [13].

The knowledge of the paramagnetic centers concentration and properties give us EPR spectra analysis. The following parameters of the EPR spectra are analysed: amplitude (A), integral intensity (I), linewidth (ΔB_{pp}), g-factor [12-14]. Amplitude increases with increasing of the amount of the paramagnetic centers in the sample. Concentration of paramagnetic centers in the samples is proportional to integral intensity. Integral intensity is obtained by double integration of the first derivative spectrum. Linewidth is effected by magnetic spin-spin and spin-lattice interactions in the sample. g-Factor depend on localization of unpaired electrons in the sample. Parameters of EPR spectra depend on microwave power (MP). The prepared didactical program presents analysis of microwave saturation of EPR spectra recorded by the use of Radiopan (Poznań) spectrometer and Rapid Scan Unit of Jagmar (Kraków) Firm. Numerical analysis of changes of EPR parameters with microwave power is tested.

The proposed tool provide users with recorded spectra for on-line analysis. The presented layout contains the EPR device software. The users, which are already familiar with the device, can migrate to the proposed solution without effort. Moreover, new users can start from simple tutorial presented at the beginning. The first element of the tool is a data spectra inquire tool (Fig. 2).

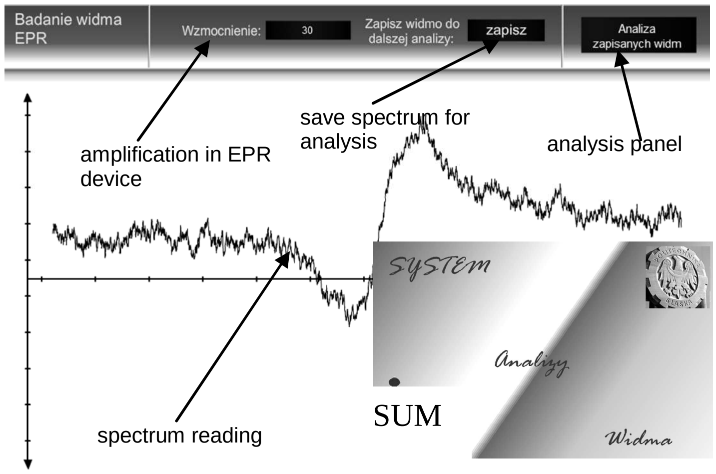

Fig. 2. Data acquire tool.

The data is acquired from the spectra storage database. In the database the data is stored as XML file sequence, indexing the experiments by the unique id. By using the id the specified XML is provided for the laboratory experiment (a) along with the data sequences of the spectra samples (b):

a)
```
<?xml version="1.0" encoding="utf-8" ?>
<settings>
    <signal pow="10">A</signal>
    <signal pow="15">B</signal>
    <signal pow="30">C</signal>
    <signal pow="35">D</signal>
    <signal pow="40">E</signal>
    <signal pow="45">F</signal>
    <signal pow="50">G</signal>
    …
</settings>
```

b)
```
SWAMP v1.0 Laboratorium EPR Uniwersytet Medyczny
Data pomiaru: 2009-05-20 10:02:05 Nazwa doświadczenia:
------------------------------------------------------
B [mT]    Uout [V]
-2.500    0.036
-2.499    0.035
-2.499    0.035
-2.498    0.032
-2.498    0.033
```

Each spectra sample is represented as a XML signal node (in *a* data file). Each signal node is described by its attributes. For radicals analysis we are using the microwave power attribute. Signal node value contains a filename of the spectra data. For methodical purposes, it is possible to add false data or set error rate to differentiate the users' analysis.

The data for analysis is represented as an discreet function *f*, and their values are defined within *b* file data. Selected spectra samples can be in the next step analysed using build up analyser. Analysis is performed in the same tool. The Fig. 3 presents its layout.

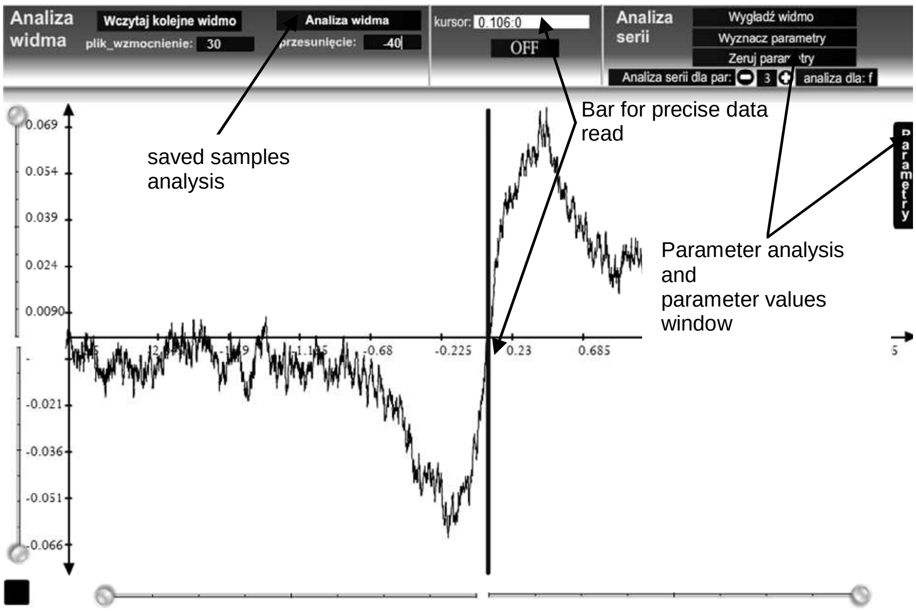

Fig. 3. Analysis tool layout.

The analysis window allows to open previously saved files. Then based on the vertical bar user can read exact values within signal sample. The bar is also used for the signal spectrum parameters' evaluation. For this purpose the analysis panel is defined. It allows to decrease the noise for the examined spectrum. The algorithm is expressed as the transformation of the discreet function *f* into *f'*, based on the area parameter ($s, s \in N$):

$$f'(x) = \frac{\sum_{i=x-s}^{x+s} f(i)}{2s+1} . \qquad (1)$$

The user can perform the noise reduction operation several times. If the result is acceptable, the next evaluation phase takes place. For each spectrum example the parameter evaluation is performed and stored as a i^{th} vector *v*. The currently supported parameters are:

- Minimum amplitude value (v_{i1}),
- Maximum amplitude value(v_{i2}),
- Amplitude range a, defined as $v_{i3}=v_{i1}-v_{i2}$,
- Left integral value ($-\infty, x_{bar\ position}$) of function ($v_{i4}$),
- Right integral value ($x_{bar\ position}, \infty$) of function ($v_{i5}$),
- Signal asymmetry *p* defined as $v_{i6}=| v_{i4} |/| v_{i5} |$.

All parameters are the result of commonly known numeric operations [11]. For the integral evaluation the trapezoidal rule were used. The generated vector is added to *E* matrix as next i^{th} row, along with the microwave power value, for the further analysis. The analysis is based on the two parameters series (two columns) of the *E* matrix (Fig. 4).

The tool helps to perform the analysis of gathered data as a function and its gradient function. The basic parameters are evaluated by the tool, however, the final evaluation is performed by the teacher, based on full user's report. Reports are uploaded by LMS platform (e.g. MOODLE).

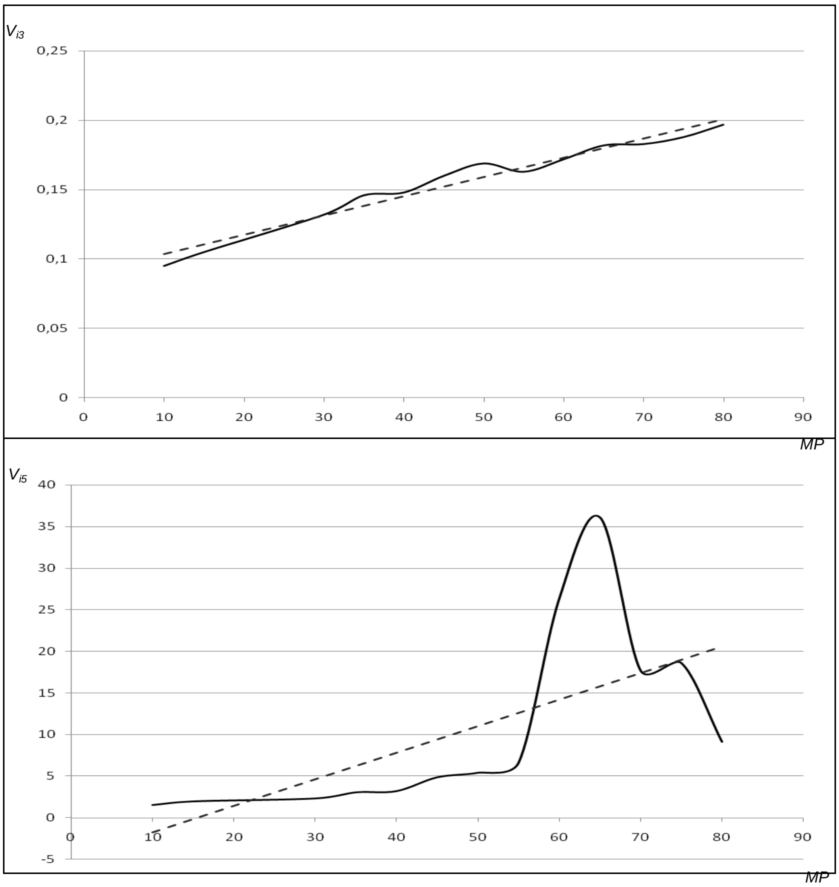

Fig. 4. Analysis tool for separate *v* parameters in power attribute function.

4. CONCLUSIONS

The proposed tool was evaluated by medical and non-medical study participants - virtual laboratory users. Given opportunities of studying at home (via virtual laboratory) were used by 95% of the laboratory students. The remaining part preferred studying in a traditional way. The students' training sessions completed the introduced experiments within 3 days (including weekend). The tool was used simultaneously by students for over 16 hours. The users' feedback and willingness of working at the virtual laboratory illustrate the references given in Fig. 5.

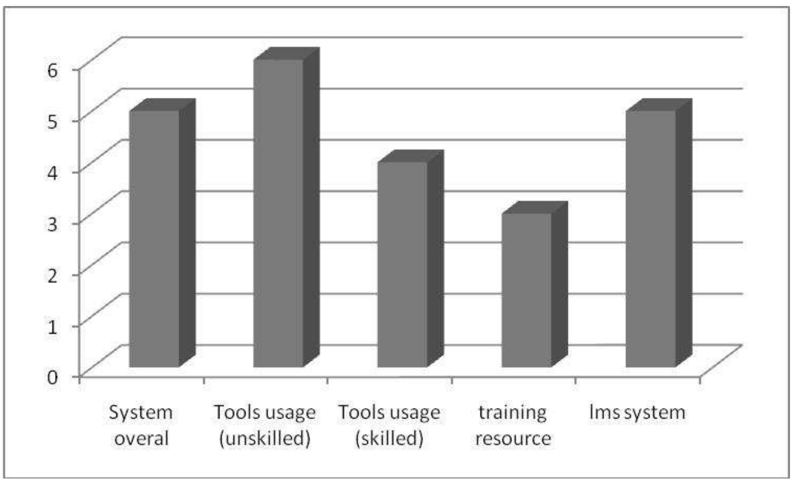

Fig. 5. The users' feedback for multiple aspects of the system in a scale from 0 to 6.

Results are very encouraging, for students not familiar with EPR device or those with vast knowledge in using it.

The students' score rate was above good. The only weak point of this solution concerns a limited range of samples provided. The indicated restrictions are relatively simple to overcome and provide analysis' tool as a very valuable training possibility.

The developed training platform is able to solve many limitations of training, using a real industrial equipment at home (e-training) as well as working by the diploma student (e-work) any time they need the machine.

The solution uses the existing laboratory infrastructure giving the students additional opportunities for improving their skills. Additional advantage of this solution concerns remarkably lower implementation costs.

Moreover, the idea illustrates changes that will be soon observed in everyday didactic processes. The laboratory can be used continuously any time it is needed.

The EPR device can be totally separated, if needed. It is a vital feature in case of the medical devices. The training facilities are defined as a feedback loop of the training complex process analysis.

The next step will concern the increase of laboratory analysis tools range as well as its adaptation for new areas of the research. The key issue is to provide an expert system as a tutor to improve users' research possibilities in the part time. The tool with the exemplary data is available at: www.science-tech.pl/proj1.

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