

## **T01. St. Petersburg State Technological University of Plant Polymers: incorporation of chemometrics into its research and educational activities**

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Saint Petersburg State Technological University of Plant Polymers (SPb STUPP), the WSC7 host, is the only higher educational establishment in Russia providing integrated training of multiskilled specialists for industrial enterprises engaged in in-depth chemical processing of wood (i.e. for the pulp and paper industry).

The use of chemometrics approach can assist in solving of a number of both industrial and scientific problems arising in pulp production and paper making. First, this industrial sector is among those where on-line automated process control together with fault detecting is important and strongly required. Being coupled with some chemometrics approach versions such as PCA, methods of fuzzy logics, neural networks, etc., the process monitoring becomes more efficient. It makes possible early detection and identification of process faults as well as their elimination at early stages, not bringing protective systems into operation and increasing thus production reliability and efficiency. This has been shown in numerous studies on the use of statistical methods in process monitoring and diagnostics carried out by Prof L. Rusinov and his colleagues. Prof. Rusinov's presentation is incorporated in the WSC 7 programme.

At the Physics Department of our university chemometrics methods find their use as a mathematical tool for interpreting FTIR spectra of different wood species and different pulps. The approach developed by scientists of the Laboratory of Spectroscopy has made possible construction of calibration models usable for fast estimation of chemical parameters, reflecting changes in major wood components caused by different treatments of wood and its constituents (such as pulping, pulp delignification and bleaching, artificial and light ageing of pulp fibers, etc.). Some results of these studies are presented in the report of Dr. O. Derkacheva. In the poster of Master's Degree student A. Dynina (Dr. Derkacheva is a supervisor) it is shown that the application of FTIR spectroscopy together with PCR makes it possible to construct models for predicting paper brightness. This approach is of considerable promise for paper restoration studies.

Chemometrics approach was also used by Department scientists for decomposing vibrational spectra of the majority of oxide glass forming systems and particularly leads metaphosphate —  $\text{TeO}_2$  glasses for the purpose to investigate intermediate-range order. Results obtained when applying factor analysis have confirmed those based on the constant stoichiometry groupings (CSG) concept. The concept has come from the finding that vibrational spectra of glasses can be interpreted as a superposition of relatively small number of unchangeable spectral forms belonging to CSGs. This concept opens the promising way for developing glasses characterized by the record Kerr coefficient and low scattering losses to be usable for Raman fiber lasers and amplifiers. These results obtained under the leadership of Prof O. Yanush will be also presented in the poster session.

The fact that chemometrics methods can be fruitfully used in research carried out in different fields of university specialization is among the reasons why it is important to include chemometrics as a

discipline into university curricula especially at the Master's level. Recognizing this, SPb STUPP is making efforts to integrate chemometrics training components into its educational process. For example, the university together with other partners: LUT, Finland, AAUE, Denmark, ICP RAS, RF, having wide experience in chemometrics education has recently implemented the project aimed at determining features and basics of a distance learning course in chemometrics for technological and natural science mastership education