Evaluation of the Research and Professional Activity of the Institutes of the Czech Academy of Sciences (CAS) for the period 2010–2014

Final Report on the Evaluation of the Institute

Name of the Institute: Institute of Analytical Chemistry of the CAS

Fields, in which the Institute registered its teams:

Chemical sciences

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Commission No. 4: Chemical sciences
Chair: Dr Habil, Academician Christian Amatore

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Programme of the visit of the Institute: see attached Minutes from the visit

Evaluated research teams:

- **Department of Bioanalytical Instrumentation**
- **Department of Electromigration Methods**
- **Department of Trace Element Analysis**
- **Department of Fluid Phase Separations**
- **Department of Environmental Analytical Chemistry**

1. Evaluation of the Institute as a whole

1. Introduction

The Institute of Analytical Chemistry (IAC) has a major mission of covering fundamental research in analytical chemistry and inventing and propagating novel analytical methodologies into fields as important as biology, medicine and environmental monitoring and protection, which have increasing demands for fast, selective and reliable analyses on smaller and smaller samples.

This mission must be recognized as being absolutely distinct from the providing of analytical services, though this is the current subject of important demands on analytical measurements that are pervading all aspects of human activities. Hence, although some other institutes of the CAS may have their own analytical directions and service functions, the focus of IAC has been in the development of cutting-edge analytical instrumentation, measurement methodologies and their conceptually important applications in key areas of science and technology.

The most recognized direction of IAC has historically been focused on separation sciences (chromatography and electrophoresis), and among the currently operating “five departments” (or rather teams), three still maintain this direction: (1) Department of Bioanalytical Instrumentation; (2) Department of Fluid Phase Separation Methods; and (3) Department of Electromigration Separation Methods. The two remaining teams, which are Trace Element Analysis and Environmental Analytical Chemistry, are thus balancing the overall analytical activities of IAC through considering goal-oriented analytical researches rather than new methodological areas. Overall, this structure roughly corresponds to the distribution of the worldwide activities in the field of analytical chemistry (except for the area of electroanalytical chemistry, which is for historical reasons, covered in Czech Republic by a different institute).

With its 49 researchers, IAC is one of the smallest institutes of CAS. The present organization and management of IAC inherently reflects some reorganizational changes since 2013 – see details below.

2. Strengths and Opportunities

The field of analytical chemistry, in general, and with chromatography, electrophoresis and mass spectrometry as its subfields, in particular, have greatly

enabled emergence of some of the most exciting science of our times such as genomic sequencing and the “omics revolution”. These activities, in turn, are currently having an enormous impact in biology and medicine, not mentioning other areas of importance for society such as traded materials certifications and fraud detection.

The analytical challenges to solve important biological questions are still substantial: (a) to deal with the extremely high complexity of proteomes, glycomes and metabolomes; (b) to enhance the measurement sensitivities to the level of single biological cell investigations; and (c) to multiplex such important measurements and develop the means to interpret complex analytical data. Continuous developments in these areas are prompted by their own successes since fulfilling an analytical challenge at a given time prompts more specific demands towards faster responses, higher selectivity and use of smaller and smaller samples.

Developing cutting-edge tools for this type of research remains to be a major goal of this Institute, which has had traditional strengths and international reputation in chromatography and capillary electrophoresis. To sustain the institutional reputation in these areas against today’s formidable competition at the international level is not easy, yet a significant progress has been achieved since the last evaluation time in the Departments of Bioanalytical Instrumentation and the Department of Fluid Phase Separations (both reorganized and enlarged in 2013). In particular, the Department of Bioanalytical Instrumentation appears to attract young talented investigators and research funds. Overall, these two research units, with their efforts in microfabrication, designs of new separation media, and miniaturized detectors and sensors are capable to sustain or even improve the institute reputation in the international arena. It appears that their 2013 reorganization has been a successful step forward. The Department of Electromigration Separation Methods has showed some incremental progress since the last evaluation. The Department of Trace Elemental Analysis remains a significant regional resource for atomic spectroscopy. It has held its steady course during the evaluation period and maintained very good research productivity. The last evaluated team (Development of Environmental Analytical Chemistry) works on seemingly important projects of the national and regional significance and maintains adequate funding. However, its overall mission was difficult to judge by the Commission from the presented materials.

Overall, the Institute represents a wide range of activities in analytical chemistry. Its extensive collaborations with other institutions are notable. The Institute is a valuable asset to CAS.

3. Weaknesses and Threats

While the individual teams show some areas of excellence, there is considerable unevenness in their performance as judged by the usual criteria as are their international reputation, the number and quality of research communications in scientific literature, and their success of attracting funds and young talented coworkers. Three out of five departments seem to have improved their performance from the situation 5 years ago: bioanalytical instrumentation and fluid-phase separations teams show notable strength and potential to compete internationally in their scientific areas, while the atomic spectrometry team seems to hold its steady state and utility as a regional resource. However, the Department of Electromigration Separations seems to have slipped away from its once distinguished research and international reputation. It likely needs a significant reorientation and increased management from above. The last evaluated team, the Environmental Analytical Chemistry, has left the Commission with a confused impression about the mission and quality of research in this team.

The global research output is acceptable, although many articles appear in very specialized journals except for some teams as noted in the individual teams' evaluations. Even though it is noted that this is often the case in analytical methodological researches elsewhere, publications in top analytical journals such *Analytical Chemistry* are encouraged rather than targeting lower-quality articles with IF often on the lower end of the scale. Similarly, the number of patents granted seems to be decreasing – with only 1 patent in 2014 – especially owing to the Institute's mission and research goals.

The cooperation with good international universities is high, but the scientific contacts with national universities appear to be contrastingly rather small with the consequence of limited outreach in education.

4. Recommendations

The above comments point out to the importance of the Institute's mission and its visibility at the national level, and at the international reputation for some of the

teams. However, several weaknesses have also been pointed out, in particular concerning the level of publications and the surprisingly low number of patents taken in view of the produced research and, for some of the teams, good and significant cooperation with instrument companies.

This, as well as some presentations, left the Commission wondering about the managerial effectiveness and direction provided at the Institute level. Indeed, this is at contrast with the fact that the Institute evidently gathers a significant number of highly qualified personnel with a good age structure of the institute (only 8 researchers over 49 have passed their 60th birthday) and ought to maintain its missions to the highest level in the future. The Committee communicated this important recommendation to the Director.

5. Evaluation of the individual teams

Evaluation of the Team: Department Of Bioanalytical Instrumentation

1. Introduction

The Department of Bioanalytical Instrumentation was created based on the fusion of two previous departments with somewhat different orientations and very different ratings in the last CAS evaluation. The incorporation of a department previously known as the Department of Proteomics and Glycomics into the new departmental structure occurred around 2013. While the modern analysis of proteins and glycoconjugates remains one of the major goals of the new scientific unit, the orientation has changed substantially: from the more application-oriented directions towards cutting-edge instrumentation research that is consistent with the analytical needs of modern biology and medicine. The orientation of the former Department of Proteomics and Glycomics was largely toward characterization of agricultural and food products; under that orientation, some scientific results were obtained and published and will thus be a part of the overall evaluation.

Current department's directions favor advancing bioanalytical techniques and exploring new technologies in micro- and nanoscale fabrications aimed to improve the performance of separation devices (new sensors and miniaturized detectors, on monolithic materials for sample enrichment, on the coupling of capillary electrophoresis and mass spectrometry, and on proteomics for cancer research). The department has built on the extensive knowledge and traditions of the Institute in analytical separation science and the related instrumentation. The leading scientists in this research unit are experienced and mature individuals who seem to lead effectively the junior scientists. The department's age distribution is very favorable. Apparently, the projects in this unit have been attractive to graduate students who decided to continue their work toward their Ph.D.s.

The department members are quite interactive with other research units in the Institute, for example, with the Department of Fluid-Phase Separations and Department of Electromigration Methods. These interactions are positively reflected in some joint publications and other scientific outputs. There are also collaborations with the academic institutions in Brno (Masaryk University and Technical University of Brno) and University of Pardubice, as well as a major collaboration with the

Biophysical Institute of CAS (Brno). Additionally, international collaborations (Hungary, Germany, Ireland, Australia, United States) complement significantly the main activities of this scientific team. This group has made very valuable contributions to organizing a highly successful conference (CECE) taking place annually in Brno.

There has been excellent outcome of the research activities from this scientific team, which is documented by publications in respectable journals and other evidence of positive scientific outputs such as participation in national meetings and international symposia. External financial support for different research projects has been outstanding. Satisfactory educational activities have been demonstrated.

2. Strengths and Opportunities

The Department of Bioanalytical Instrumentation was highly rated in the previous evaluation period and continues its excellent record of accomplishments during this period. Drawing from the knowledge of “classical” capillary electrophoresis (CE) and its instrumentation, significant progress has been made toward developing unique microfabrication technologies for CE separation channels on microchips. Perhaps the most important avenue toward tapping the potential of CE separations has been development of detection techniques (miniaturized detectors). This appears to be a long-term goal of the researchers in the field worldwide to which the members of this department are responding in some unique ways. This includes, perhaps most importantly the thus far elusive goal of combining effectively CE with mass spectrometry (MS). The CE-MS interfacing has been a major project in this group of scientists. While progress in this field has been thus far incremental, this team has become one of the leading groups to tackle this ostensibly difficult problem and seems poised to make further improvements through unique instrumental designs. Besides CE-MS, there are other detection opportunities for CE and miniaturized chromatography. This team has pursued some of them with very promising results: contactless conductivity detection; fluorescence detection; immunodetection with conjugated quantum dots; and surface-enhanced Raman spectroscopy. This highly talented team is likely to come up with new ideas in a very important field, and they should be encouraged to do so. During the well-organized presentation, additional progress (i.e., beyond the written report) has been demonstrated concerning the miniaturized and highly sensitive detectors and sensors. The local facilities and

collaborative efforts in microfabrication seem on the right target in developing new separation-based analytical strategies.

The international cooperation with very high-ranking international universities and research institution is very good. As is the cooperation with instrument companies, which is clearly of high importance in a fundamental research effort prone to lead to important applicative outcomes.

Modern biology and medicine are inspirational fields for future developments of powerful bioanalytical tools. This team seems to have recognized this fact in their current and proposed activities. Their instrumental and detection developmental activities are geared toward improvements in proteomic and glycomic analyses: development of capillary enzyme reactors; fluorescence and cationic labeling of oligosaccharides; measurements at the level of single biological cells; and phosphopeptide enrichment.

Additional strong features of this research team are in clever exploring of microfabrication and nanotechnologies such as creation of solid mercury amalgam microelectrodes for protein electrochemical measurements and the use of nanoparticles in analyte preconcentration and spectroscopic measurements. (It is noted that solid mercury amalgams increase electrochemical performance without presenting contamination risks due to mercury metal and salts' disposal). Continued efforts in these areas should be encouraged.

3. Weaknesses and Threats

No particular weaknesses or threats were evident to the Commitee. The team is highly productive (though it is noted that this was not stressed efficiently during the on-site visit) and has a healthy balance of different projects in the mainstream of bioanalytical chemistry, substantial financial support through 2018, and a favorable age distribution.

However, the leadership will face a delicate task of reassigning different projects to the scientists from the team terminated in 2013 and integrated in the present Department. It is noted, in this respect, that some concerns expressed by the commission concerning this point were addressed. As an example of the renewed proteomic analysis opportunities, a collaboration with the Slovak Academy of Sciences in cancer research has been demonstrated through two recent publications.

4. Recommendations

The Commission fully endorses the scientific directions of this team and the plans for research and increased orientation of new analytical tools toward the solution of problems in contemporary biology and medicine. Besides the proposed in-house facilities for biological cell cultures, increased attention will be needed toward cell sorting, preconcentration and the analyses of subcellular entities. Some of these activities could ideally be covered in collaboration with the Department of Fluid Phase Separations.

Finally, we fully endorse this team's involvement in organizing the successful series of CECE meetings as well as their role in planning the HPLC 2017 Symposium in Prague. These activities contribute greatly to international scientific interactions while enhancing the institutional prestige and recognition.

5. Detailed Evaluations

In accordance with the oral presentation, this Department divides into four different directions: (a) sensors and miniaturized detectors for CE or LC; (b) development of sample enrichment strategies and microreactors; (c) coupling CE with MS; and (d) proteomics for cancer research. These all represent the long-term objectives in biochemical analysis. The team has been able to archive significant results publishable in respected analytical literature. The senior researchers are well-recognized nationally and even internationally for some of them. The students' participation in this research program has been excellent. Development of new biomedically relevant measurement technologies has high societal importance by fulfilling increasing needs in diagnostic and prevention based on biological samples of decreasing sizes.

There is a significant potential for the main project areas and, given the favorable age distribution, the basis for sustainability. The benefits of the fusion of two different teams in 2013 are still to be clearly seen, but the initially successful entrance into the cancer-related collaboration is viewed optimistically.

Evaluation of the Team: Department of Electromigration Methods

1. Introduction

Electromigration methods have a long tradition and distinguished record of accomplishments at the Institute in Brno. The early involvement in isotachophoresis (ITP) research at the Institute was further strengthened during the 1980s due to the advent of capillary zone electrophoresis (CZE) and its rapid commercialization in the Western countries. The research group around Petr Bocek responded to the opportunities of this rapidly evolving field so that capillary electromigration techniques became a major research area in the Institute. Accordingly, the group has held its significant international reputation for a long time and had an important role within the Institute. However, since the Department of Electromigration Methods has made the choice to hold a somewhat “steady course” throughout the period for this evaluation, interest in capillary electrophoresis (CE) has become no longer its exclusive domain in the Institute. At least two other departments in the Institute are also involved with electromigration techniques, albeit at different angles.

The Department of Electromigration Methods has traditionally covered a wide range of research activities: from theoretical aspects of electrophoresis to instrumentation to unique applications. This has also been the case during this period as well as with the projections into the near future. The current team is relatively productive, but the questions arise as to whether its “steady course” will remain justified due to its unfavorable age distribution, funding uncertainties, and little input from graduate students at present. In the latter case, the team outreach into education is not very large despite the high demand on technicians and doctors with adequate training in advanced separation methods as this team is expected to provide.

2. Strengths and Opportunities

The department and its leading scientists have been internationally known for their efforts to understand and analytically exploit electromigration stacking behavior taking place in isotachophoresis (ITP). Both theory and experimental elucidation efforts of this team have been clearly recognized in the relevant literature. The team has had a great knowledge of the electrolyte systems and the means to influence migration of studied analytes for benefits of trace analysis. While using both

computer stimulations and selected CE measurements, important predictions can be made toward optimum analyses of certain sample components. Whereas ITP has not become a truly multicomponent analytical technique, when compared to CZE, it has strengths in sample preconcentration, as demonstrated by several applications to trace analysis by this team. The combination ITP/CZE has been explored to some extent. Acquisition of mass spectrometry in 2010 has allowed the team to explore different aspects of ITP/MS combination, particularly a selection of suitable buffers for the CE-MS measurements. Perhaps the most novel research direction of this team has been the use of supported liquid membranes and other microextraction techniques for biological materials through electromigration. In general, the research of this team shows a sound interplay of fundamentals and their applications in trace analysis. However, all applications are confined to analyses of relatively small ions, leaving out some great opportunities to study biomolecules through their approaches
.

3. Weaknesses and Threats

While this department has had a long and distinguished history in the area of electrophoresis, there are now some signs of incomplete leadership and maturation of the field. Although its current publication record appears satisfactory, a significant number of articles are of a minireview and tutorial quality rather than original communications. The description of future plans reflects no significant departure from the *status quo*. While the senior members of this team hold positions on editorial boards and there are satisfactory pedagogical activities, the presence of the team researchers at major international symposia decreased substantially compared to the previous years. The age distribution chart indicates problems of attracting younger researchers to the field in contrast with the usual career request for young technicians and Ph.D.s.

The funding situation does not appear favorable; in fact, it is, surprising that the team’s activities could be sustained through the 2010-2014 period when most of the grants expired earlier.

4. Recommendations

To become once again competitive at the international level, the department should thoroughly re-evaluate its goals for future and implement an adequate strategy in line

with the strategies decided at the level of the Institute. This is essential for capitalizing on the team's significant knowledge and reputation and for advancing these qualities back into the mainstream of the field and new analytical needs. The selected applications and their current research in miniaturized membrane extractions and preconcentration are promising, but these alone are unlikely to guarantee sustainability of this team in a longer run. Perhaps most importantly, recruitment of young talented researchers should have highest priority.

5. Detailed Evaluations

The quality of research in this department is satisfactory, but not outstanding. While progress has been made in understanding and optimization of electrolytes in ITP and CZE, the results are largely incremental. The acquisition of a mass spectrometer instrument improved significantly the analytical capabilities of this team, as demonstrated by the applications demonstrating selective detection of trace components in highly complex sample matrixes (e.g., fungicide in orange juice and analgesics in waters, both at the level of nanogram per liter). Some of the more promising applications to the analysis of crude samples, such as physiological fluids, involve the use of supported liquid membranes that can be directly coupled to CE (including its pairing with different commercial instruments). Some demonstrated applications of CE, such as environmental analyses or clinical determinations, rapid diagnosis of methanol poisoning, etc., have significant societal relevance. A systematic search for selective preconcentration techniques prior to CE is a worthwhile research to do. The department is interactive at the regional level (Masaryk University, Mendel University of Agriculture, and Technical University of Brno). Its international reputation is considerably less than in the previous years. Unless this is promptly rectified, a further decline is highly probable.

Evaluation of the Team: Department of Trace Element Analysis

1. Introduction

The Department of Trace Element Analysis augments the analytical chemistry fields in Brno, representing the field of atomic spectrometry. The Team mission focuses on the development and testing of new methods for trace and ultratrace elemental analysis in complicated matrices (as e.g. in biological samples) taking advantage of its expertise in atomic spectroscopy methods (AAS, AFS or ICP-MS) and in preconcentration techniques for researches focused mainly towards biomedical and environmental fields.

While this team is physically located in Prague, on the campus of biological/medical institutes of AS CR in Krc, it is administratively a part of the Institute in Brno and interacts somewhat with the Department of Environmental Analytical Chemistry of the Institute. It has also a significant role in its connection to Charles University in Prague, covering the educational activities in the field of atomic spectrometry (lectures and laboratory instruction). Whereas the field has reached a substantial maturity in terms of fundamental instrumentation development, a state-of-the-art research and service team with a considerable knowledge of the field is a significant asset to the CAS and indeed regionally. There are still many applications of environmental and biomedical interest worth pursuing. To do so, the Department is relatively well equipped with the ICP-MS, atomic absorption, atomic fluorescence, etc., instruments (mostly purchased relatively recently).

The relative maturity of the field seems to reflect a quite small group of investigators (7 researchers totalizing ~5 FTE consisting of generally rather young permanent staff providing a reasonable age structure in the team), and mostly M.S. degree students, but a very few Ph.D. students. Nevertheless, this team has been quite productive as reflected in the publications in *Analytical Chemistry* and some more specialized journals, as well as by some patents. Their participation in international collaborations has been visible.

As stated above, the major mission of this research unit is to develop optimum measurement techniques for trace-elemental and speciation analysis, but their effective applications to samples of environmental and toxicological interest are

important as well. Besides the wide-ranging applications of the trace elemental analysis, the team has concentrated on some troublesome aspects of arsenic speciation, generation of volatile species for transition metals, and some aspects of sample preconcentration. Their unique instrumental ("front-end") abilities deal with investigation of novel atomizer techniques, in particular on the so-called dielectric barrier discharge plasma.

The team has been adequately funded during the evaluated period, evidencing the interest of its methods within the general scientific national background.

2. Strengths and Opportunities

The speciation of the "difficult element" (arsenic) is a toxicologically important subject where this group has already obtained some proficiency and recognition, as evidenced by the publications in high-impact journals (Analytical Chemistry, and Chemical Research in Toxicology). They have developed unique approaches to reach high sensitivity (selective hydride generation/cryotrapping prior to the measurements) and should take advantage of their capabilities before competing groups elsewhere become more intensely involved. The determination of arsenic-containing metabolites in biological tissues and the foodstuff we consume is likely to remain a "hot subject" for some time. Further investigation of the atomization for transition trace metals also appear in order. While the international collaborations and student exchanges appear to be a very healthy aspect of this research program, the Commission highly recommends promoting a closer contact with the biological institutes on the Prague-Krc campus, and potentially, with the new biomedical center in Vestec. It is, however, necessary that biologists and medical scientists become more aware of the state-of-the-art capabilities in the measurements of trace bioelements as well as different toxic species, so that some "education" or advocacy by this team might be necessary among scientists of other fields. Conversely, the team outreach into education – including high school education – appears good, as is visible in the number of MS and BS students working with the Team.

Based on his expertise, the team has developed good and established foreign collaborations, and achieved a good visibility in its field in a world context.

Finally, it is noted that up to now the Team has been able to secure enough grant money. It is noteworthy that some funds were granted by international organizations.

3. Weaknesses and Threats

Although this team has been productive and recognized nationally and internationally, the field of atomic spectroscopy has been maturing rapidly. Short of some unexpected breakthrough developments, there is a great need to become more of the problem-solving facility with less emphasis on technique-oriented research. In this respect, while the Team's physical separation from its Institute could bring administrative problems, its location on a campus where all other institutions are working in biological and medical fields may be turned into a unique scientific advantage for dissemination of their specialized expertise and instrumental methods.

Contrastingly, it is noted that if the research proposed for the next period will provide continuity, it will probably carry no significant innovations in methodology. This is also related to the acknowledged lack of interest on the part of doctoral students in this field. Eventually, this may also influence long-term conditions in funding and sustainability.

4. Recommendations

This department has acquired substantial expertise, instrumentation and the knowledge base to serve as a regional resource in atomic spectroscopy. Continuation of their work in solving the problems of arsenic speciation is highly important. Other planned projects involving new technologies for preconcentration, volatililization and atomization concerning other trace elements are also desirable. It is highly recommended by the commission that this team utilizes more effectively their geographical proximity with the biologically- and medically-oriented teams on the Krc campus to develop win-win collaborative arrangements. The Team should take advantage of the creation of the BIOCEV research center to stimulate interest mainly in trace metal analysis among biologists and close hospitals.

5. Detailed Evaluations

The overall scientific output of this team is at least adequate, with more than 30 papers published during the period under evaluation. While several papers appear in high-impact journals (e.g. Analytical Chemistry), most publications appear in specialized journals. While the general pedagogical activities of the team are substantial, the involvement of students in research activities is only moderate. This is surprising since several team members are regularly teaching, mainly in Charles

University in Prague and, thus, have regular contacts with students. Furthermore, it is noted that over the evaluation period, the Team members were supervisors of a number of BSc, MSc or Ph.D. thesis including the supervision of students studying at foreign universities. The reasons for this odd situation should be analyzed with care and remediated.

This department has an important role as a regional resource in atomic spectrometry and its societal relevance is high because of its activities in environmental and toxicological analysis. The research toward the development of better techniques for arsenic speciation measurements is a good example of societal relevance. This team is quite interactive internationally and in cooperation with other universities at the national level.

A continued vitality and sustainability at the current level appear reasonable. In terms of future plans and strategies, the management of CAS should evaluate the role of this team in a close cooperation with the biological and medical institutes in Krc. Indeed, the Team research field seems to be somewhat matured but new impulse should be infused, possibly through encouragement of its younger collaborators and external collaborations. As mentioned in presentation, the Team should look for possibilities to employ at least one skilled technician.

Evaluation of the Team: Department of Fluid Phase Separations

1. Introduction

The Department of Fluid Fluid Phase Separations is a relatively large unit in the Institute and consequently presents a large but somewhat heterogeneous spectrum of research projects and to a relatively large number of publications. Its scientifically heterogenous character can be traced to the fact that it was created in 2013 through a fusion of two units with a very different scientific orientations and expertise (as per the previous evaluation). Consequently, the progress report at this date spans the subjects from the physico-chemical measurements of compound solubilities under different phase equilibria to instrument designs for capillary chromatography and isoelectric focusing, to the analysis of microorganisms and intact cells.

To their credit, the members of this integrated team have understood the danger of the team heterogeneous composition and have now learned to extensively collaborate and publish together, seeking new directions in microcolumn separations and their conceptually important applications. This team also covers a still important field of separation science – chemical aspects of chromatographic column technologies. While this team covers a considerable range of scientific subjects at present, the proposed directions indicate a more distinct focus in future. Among the developments catalyzing a closer collaboration within the team, and the Institute at large, seems to be a discovery of Michal Roth's group that the near-critical and supercritical water can be utilized to modify various separatory channels (siliceous capillaries as well as microfabricated structures) for the benefits of instrumental analyses. This novel approach deserves further explorations in future studies, in particular to explore its practical value beyond the laboratory scale.

While the team is relatively large, it shows a biphasic age distribution with a low proportion of doctoral students.

This team's scientific productivity is respectable, with numerous scientific outputs and good publication record reflecting the wide research project number as mentioned above. They have secured relatively good funding record during the current period, although the grant success is quite variable with respect to different projects.

Within the Institute, the team is scientifically interactive, as is with other institutions. The contributions of team's researchers to the scientific community are at least satisfactory. The outreach activities and research popularization for the public are also notable.

2. Strengths and Opportunities

The two teams that were merged in 2013 had previously followed the lines of research that were scientifically sound, albeit not widely recognized as the mainstream directions in analytical chemistry: (a) the use of capillary supercritical chromatography and extraction for the benefit of physicochemical measurements; and (b) isoelectric focusing of biopolymers. These were both long-standing activities in the Institute, and while there was never any compelling reason to phase out these activities, their modernization was in order during the previous evaluation period.

Through the reorganization, a visible integration of scientific activities has been shown. There are now three main recognizable trends within this team: (a) improvement in the design and scope of isoelectric focusing (IEF) methodologies and their new conceptually important applications in separating biopolymers and microorganisms; (b) new technologies in the preparation of monolithic stationary phases; and (c) analytical uses of compressed fluids. During the 2010-2014 period, the IEF instrumental studies advanced considerably in exploring both the analytical and micropreparative uses of these technologies. The collaborations with the researchers in the other institutions in the life sciences area are notable applications of the IEF techniques developed in this department. The miniaturized LC instrumentation and the monolithic column technologies are important to retain and improve for the benefits of the Institute as a whole. The proposed use of these technologies in portable analytical equipment appears desirable, however, no concrete examples were given for the benefit of this review. The use of a uniquely constructed high-pressure equipment toward the modification of microfabricated separatory channels has been innovative and exciting, deserving further explorations into the near future. Modest extensions of the previous research in supercritical fluid thermodynamic measurements still appear justified.

Whereas the research activities have been adequately funded during the past period, the departmental leadership should secure more even funding of different projects during the new period. In particular, it is noted that in spite of the nature of measurements developed by this team, there is no support by the EU.

3. Weaknesses and Threats

While this department represents a wide range of activities at the heart of analytical separation methods, its long-term activities must maintain a proper balance between the instrumental development and applied aspects of the field. Whereas the innovations pertaining to the use of near-critical water for unusual surface treatments and microfabrication have catalyzed increased collaboration within this team, it is now important to explore and develop further directions to take advantage of the Institute's unique expertise and high-pressure capabilities.

The integration of two smaller departments into a larger structure in 2013 seems to have been a very positive step. Now, with a large group of mature scientists and somewhat incremental plans for future research, it will be essential to bring more junior enthusiastic coworkers (graduate students) who can enrich the program and sustain its scope into future years.

4. Recommendations

The key scientific workers in this department have made notable contributions to scientific literature and participated in numerous conferences at both the national and international levels. Most publications have been in scientific journals with respectable impact factors, but given the number of scientists in this team, publication record should improve. International collaborations may also be enhanced. The team should more clearly define its long-term objectives. Perhaps most importantly, there is a need for active recruitment of younger investigators.

5. Detailed Evaluations

The overall quality of results obtained in the Department of Fluid Phase Separations is very good and comparable to the achievements of established laboratories elsewhere. The efforts unifying the instrumental aspects of isoelectric focusing with the applications to different separations and characterization of microorganisms (often augmented with MALDI-TOF analyses) are excellent and relevant to society (clinical microbiology, human health, food safety, agricultural production, etc.). A very

significant innovation in the department has been the realization that the near-critical and supercritical water can be used to modify geometrically and chemically the surfaces of separation channels. Unique applications of this technology were already shown with promising results for future activities. The research reported in the areas of LC instrument miniaturization and monolithic column technologies largely complements the efforts of other laboratories and are not very original. However, this general area needs to be sustained for the overall institutional benefits. Here the obvious societal importance resides with construction of portable analytical instruments, but no plans in this direction are given in the written report. This deficiency was somewhat remedied during the oral presentation by suggested applications. Supercritical fluid and pressurized-liquid extraction technologies, which were previously at the heart of the Department of Separations with Compressed Fluids, produced results with both theoretical and practical value (e.g., thermodynamic investigations in carbon dioxide/ionic liquid systems, solubilities in pressurized hot water, and pressure –assisted extractions of plant materials). These latter efforts will be gradually phased out during the forthcoming period.

The department's international interactions appear moderate as seen in 2 joint publications with a group in Finland and cooperation with Food Research Institute in Slovakia on the pressurized-fluid applications. Two researchers underwent scientific training in the United States, with notable results in proteomics and cardiovascular biomarker discovery. How will this expertise be utilized in the future plans of the department? While the department counts a high number of mature researchers, the number of students seems relatively low. Unless this becomes rectified in the near future, the vitality of this team and sustainability may become compromised. The future plans mostly reflect incremental developments in the already existing projects.

Evaluation of the Team: Department of Environmental Analytical Chemistry

1. Introduction

The main scientific activities of the team focus on the development of new methods (separation and preconcentration techniques coupled to specific detectors) and the instrumentation for the chemical analysis and/or characterization of toxic compounds in environment, which involve minor and trace gaseous components, nanoparticles and aerosols in air, and composition of nanoparticles. Environmental systems involve air, aquatic systems, soils and sediments. The teams investigates also accumulation of nanoparticles in organs after inhalation; this topic is investigated based on synthesized nanoparticle oxides using mouse models and analytical measurements of metals.

This team has presently an aggregate number of 6.0 researchers. Two of its members are above 60 years of age but 3 between 30 and 35, and only 1 graduate student.

2. Strengths and Opportunities

These research projects often involve collaboration with other research institutes, for example the defense establishment in the case of detection of RDX in soils, or a consortium of atmospheric particle scientists across the US and Europe. This is a strength of the department and offers significant opportunities for the future. An additional strength is the importance of this type of analytical chemistry, and the societal relevance of research work in this area. This is a field which is growing in importance, and should be very attractive to students and energetic young researchers who wish to impact the needs of the society. Facilities and instrumentation available for the work of the department appear to be strong.

The national role of this team is exemplified by its success in obtaining grants (5 from Czech SF, 4 from Ministry of Environment, and surprisingly, none from CAS) and by its association in the national Centre of Excellence (Centre for studies on toxicity of nanoparticles), its involvement in the preparation of the new strategy of CAS about energy, as well as by its cooperation with the Ministry of Defense for fast analysis of explosives in environment (portable detector for nitrate in water). It is also involved in a Mediterranean network (CEAM) for sensitive detection of nitrous acid in air

3. Weaknesses and Threats

A significant weakness is the age structure of the department, with very few young or mid-career researchers involved in the work of the department. The department leader, Dr. Vecera, is close to the end of his career, and new leadership should be identified and brought on board. Most importantly, the team leader did not (was not able to) make a reasonable presentation of the work of the department results and plans. This resulted in an interminable confused monolog, involving poor, often unreadable slides mixing emphasis on minor specialized details with extremely broad insufficient information about the specificities of the researches performed. This was aggravated by difficulties in using the English language and the disregarding of the Committee member's and Chair's questions aimed to help focusing the presentation that, finally, had to be interrupted by the Chair after several admonitions. This surely limits the international impact of the work of the department.

Hence, the originality of the contributions of the team was almost impossible to assess based on the written document and, as said above, the on-site presentation did not help. Indeed, even if the applications of methods and procedures are reported, it is impossible to evaluate whether they are original ones or simple adaptations of usual ones to environmental and health targets whose importance is defined by agencies rather than by scientific challenges.

The publication rate (25 articles in peer-reviewed journals) appears extremely low for a group of this size, especially in view of the large number of contributions to proceedings (61), a fact that is surprising in view of the "blooming" of the fields covered by the team in top literature anywhere across the world. The articles of the group largely appeared in accepted, but not first rate journals. This is surprising since the topics studied are of high present societal and environmental relevance.

4. Recommendations

The group clearly covering issues that, based on the number of grants obtained, are judged of importance by the Czech agencies in the fields of environment and health related to anthropic chemicals and nanoparticles. However, it is clear that the true research outcome does not go at par with the amount of grants received and that should be remediated if the team has to be considered as a research team rather than a public team offering services in answer to national calls.

The ongoing collaborations with other institutes and agencies are a strength, and should be continued and expanded if possible. Very few students and young researchers are involved in the work of this department.

There are some concerns about the design of specific projects that will be mentioned in the detailed evaluation below.

In conclusion, it is recommended that a new team leader be identified, and brought on board soon. This has been clearly stated to the Director of the Institute of Analytical Chemistry of the CAS, so that the Committee considers that the Director should take appropriate decisions.

5. Detailed Evaluation

Overall, the quality of the research results of this department and their focus appear good on the national scale. No results of international prominence or world leading character have been recently published. By far the majority of the work of this department is published in the Czech language, with a few international journals (Talanta, Atmospheric Environment) appearing in the publication report from the past five years though numerous proceedings are reported.

The significance of many results presented was extremely hard to evaluate despite they involved high investment (personnel, space, equipment). This is perfectly exemplified by the presentation of the studies related to nano-particle inhalation by laboratory animals. Although their outcome could be impressive to a general public audience, their significance was modest and maybe misleading because there were particularly poorly planned. The particulate concentrations were much higher (by a factor of ten) than even the highest naturally occurring particulate concentrations in the atmosphere. In addition, no valid controls were performed (mortality of unexposed test animals for example), nor were any studies of disease progression or organ morphological studies included. The instrumentation developed in this project could be useful in further, more well planned studies.

In contrast, the work on detection of explosive markers in soil is of significant importance and could have broader impact provided it does not suffer the same planning weaknesses as that about nanoparticles inhalation (the Committee members' expertise on this particular field was not sufficient to asses this matter).

There have also been significant contributions to the development of instrumentation and methods for detection of trace environmental contaminants, as well as instrumentation for nanoparticle toxicology assessments.

As noted above, very few students and young researchers are involved in the work of this department. This must be improved, as this is the lifeblood of a research program.

The societal relevance of the work carried out by this department is quite high. This should be a considerable strength of the department. The development of instrumentation and protocols for identifying and quantifying a range of trace contaminants in soil, atmosphere, water, and particulate materials is crucial to the characterization of the environment, and to developing ways to maintain and enhance the quality of the environment. This is an important result and continuing goal of this department, and should be encouraged provided that the work is carefully planned in view of the real environmental and healthcare demands.

The work of this department is well funded by national research funding agencies, including the Defence Ministry as well as basic research funding sources. The work on environmental toxicology is of broad and increasing interest, and is therefore highly attractive to funding agencies. There is perhaps a need to broaden the range of seriously planned projects, and to think further ahead in terms of sustainability of the efforts of this department. The proposed future work in the department is mostly more of the same as what is now being done. The work should be expanded, and not rely just on more of the same.

Date: December 26, 2015

Commission Chair: Dr Habil, Academician Christian Amatore