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Chapter 1 : Estimation of Measurement Uncertainty in Chemical Analyses | University of Tartu

Course introduction. This is an introductory course on estimation of measurement uncertainty, specifically related to chemical analysis (analytical chemistry).

For example, the measurand might be the size of a cylindrical feature, the volume of a vessel, the potential difference between the terminals of a battery, or the mass concentration of lead in a flask of water. No measurement is exact. When a quantity is measured, the outcome depends on the measuring system, the measurement procedure, the skill of the operator, the environment, and other effects. The dispersion of the measured values would relate to how well the measurement is performed. Their average would provide an estimate of the true value of the quantity that generally would be more reliable than an individual measured value. The dispersion and the number of measured values would provide information relating to the average value as an estimate of the true value. However, this information would not generally be adequate. The measuring system may provide measured values that are not dispersed about the true value, but about some value offset from it. Take a domestic bathroom scale. Suppose it is not set to show zero when there is nobody on the scale, but to show some value offset from zero. Measurement uncertainty has important economic consequences for calibration and measurement activities. In calibration reports, the magnitude of the uncertainty is often taken as an indication of the quality of the laboratory, and smaller uncertainty values generally are of higher value and of higher cost. See Joint Committee for Guides in Metrology. Indirect measurement[edit] The above discussion concerns the direct measurement of a quantity, which incidentally occurs rarely. For example, the bathroom scale may convert a measured extension of a spring into an estimate of the measurand, the mass of the person on the scale. The particular relationship between extension and mass is determined by the calibration of the scale. A measurement model converts a quantity value into the corresponding value of the measurand. There are many types of measurement in practice and therefore many models. A simple measurement model for example for a scale, where the mass is proportional to the extension of the spring might be sufficient for everyday domestic use. Alternatively, a more sophisticated model of a weighing, involving additional effects such as air buoyancy , is capable of delivering better results for industrial or scientific purposes. In general there are often several different quantities, for example temperature , humidity and displacement , that contribute to the definition of the measurand, and that need to be measured. Correction terms should be included in the measurement model when the conditions of measurement are not exactly as stipulated. These terms correspond to systematic errors. Given an estimate of a correction term, the relevant quantity should be corrected by this estimate. There will be an uncertainty associated with the estimate, even if the estimate is zero, as is often the case. Instances of systematic errors arise in height measurement, when the alignment of the measuring instrument is not perfectly vertical, and the ambient temperature is different from that prescribed. Neither the alignment of the instrument nor the ambient temperature is specified exactly, but information concerning these effects is available, for example the lack of alignment is at most 0. As well as raw data representing measured values, there is another form of data that is frequently needed in a measurement model. Some such data relate to quantities representing physical constants , each of which is known imperfectly. Examples are material constants such as modulus of elasticity and specific heat. There are often other relevant data given in reference books, calibration certificates, etc. The items required by a measurement model to define a measurand are known as input quantities in a measurement model. The model is often referred to as a functional relationship. The output quantity in a measurement model is the measurand. Formally, the output quantity, denoted by Y , about which information is required, is often related to input quantities, denoted by X.

Chapter 2 : Measurement uncertainty

The author considers issues covered by A.B. Blank in his letter "Uncertainty in Measurements and Chemical Analysis" published in Zhurnal Analiticheskoi Khimii in (vol. 60, no. 12, p.).

Gustav Kirchhoff left and Robert Bunsen right Analytical chemistry has been important since the early days of chemistry, providing methods for determining which elements and chemicals are present in the object in question. During this period significant contributions to analytical chemistry include the development of systematic elemental analysis by Justus von Liebig and systematized organic analysis based on the specific reactions of functional groups. The first instrumental analysis was flame emissive spectrometry developed by Robert Bunsen and Gustav Kirchhoff who discovered rubidium Rb and caesium Cs in During this period instrumental analysis becomes progressively dominant in the field. In particular many of the basic spectroscopic and spectrometric techniques were discovered in the early 20th century and refined in the late 20th century. Starting in approximately the s into the present day analytical chemistry has progressively become more inclusive of biological questions bioanalytical chemistry , whereas it had previously been largely focused on inorganic or small organic molecules. Lasers have been increasingly used in chemistry as probes and even to initiate and influence a wide variety of reactions. The late 20th century also saw an expansion of the application of analytical chemistry from somewhat academic chemical questions to forensic , environmental , industrial and medical questions, such as in histology. Many analytical chemists focus on a single type of instrument. Academics tend to either focus on new applications and discoveries or on new methods of analysis. The discovery of a chemical present in blood that increases the risk of cancer would be a discovery that an analytical chemist might be involved in. An effort to develop a new method might involve the use of a tunable laser to increase the specificity and sensitivity of a spectrometric method. Many methods, once developed, are kept purposely static so that data can be compared over long periods of time. This is particularly true in industrial quality assurance QA , forensic and environmental applications. Analytical chemistry plays an increasingly important role in the pharmaceutical industry where, aside from QA, it is used in discovery of new drug candidates and in clinical applications where understanding the interactions between the drug and the patient are critical. Classical methods[edit] The presence of copper in this qualitative analysis is indicated by the bluish-green color of the flame Although modern analytical chemistry is dominated by sophisticated instrumentation, the roots of analytical chemistry and some of the principles used in modern instruments are from traditional techniques, many of which are still used today. These techniques also tend to form the backbone of most undergraduate analytical chemistry educational labs. Qualitative analysis[edit] A qualitative analysis determines the presence or absence of a particular compound, but not the mass or concentration. By definition, qualitative analyses do not measure quantity. Chemical test There are numerous qualitative chemical tests, for example, the acid test for gold and the Kastle-Meyer test for the presence of blood. Flame test Inorganic qualitative analysis generally refers to a systematic scheme to confirm the presence of certain, usually aqueous, ions or elements by performing a series of reactions that eliminate ranges of possibilities and then confirms suspected ions with a confirming test. Sometimes small carbon containing ions are included in such schemes. With modern instrumentation these tests are rarely used but can be useful for educational purposes and in field work or other situations where access to state-of-the-art instruments are not available or expedient.

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Chapter 3 : Analytical chemistry - Wikipedia

*Measurement Uncertainty in Chemical Analysis [Paul De BiÃ¨vre, Helmut GÃ¼nzler] on calendrierdelascience.com *FREE* shipping on qualifying offers. It is now becoming recognized in the measurement community that it is as important to communicate the uncertainty related to a specific measurement as it is to report the measurement itself.*

The concept of measurement uncertainty MU Brief summary: This section introduces the concepts of measurand, true value, measured value, error, measurement uncertainty and probability. The concept of measurement uncertainty https: The quantity that we intend to measure is called measurand. In chemistry the measurand is usually the content concentration of some chemical entity molecule, element, ion, etc in some object. The chemical entity that is intended be determined is called analyte. Measurands in chemistry can be, for example, lead concentration in a water sample, content of pesticide thiabendazole in an orange or fat content in a bottle of milk. In the preceding example lead element , ascorbic acid molecule and fat group of different molecules are the analytes. Water, orange and milk are analysis objects or samples taken from analysis objects. In principle, the aim of a measurement is to obtain the true value of the measurand. However, our measurement result will be just an estimate of the true value and the actual true value will almost always remain unknown to us. Therefore, we cannot know exactly how near our measured value is to the true value â€" our estimate always has some uncertainty associated with it. The difference between the measured value and the true value is called error. Error can have either positive or negative sign. Error can be regarded as being composed of two parts â€" random error and systematic error â€" which will be dealt with in more detail in coming lectures. Like the true value, also the error is not known to us. Therefore it cannot be used in practice for characterizing the quality of our measurement result â€" its agreement with the true value. The measurement uncertainty U itself is the half-width of that interval and is always non-negative. The symbol U is picked on purpose, because expanded uncertainty generally denoted by capital U fits very well with the usage of uncertainty in this section. However, it is not explicitly called expanded uncertainty here, as this term will be introduced in later lectures. The following scheme similar to the one in the lecture illustrates this: Interrelations between the concepts true value, measured value, error and uncertainty. Measurement uncertainty, as expressed here, is in some context also called the absolute measurement uncertainty. This means that the measurement uncertainty is expressed in the same units as the measurand. As will be seen in subsequent lectures, it is sometimes more useful to express measurement uncertainty as relative measurement uncertainty, which is the ratio of the absolute uncertainty Uabs and the measured value y: Measurement uncertainty is different from error in that it does not express a difference between two values and it does not have a sign. Therefore it cannot be used for correcting the measurement result and cannot be regarded as an estimate of the error because the error has a sign. Instead measurement uncertainty can be regarded as our estimate, what is the highest probable absolute difference between the measured value and the true value. With high probability the difference between the measured value and the true value is in fact lower than the measurement uncertainty. However, there is a low probability that this difference can be higher than the measurement uncertainty. Both the true value and error random and systematic are abstract concepts. Their exact values cannot be determined. However, these concepts are nevertheless useful, because their estimates can be determined and are highly useful. In fact, as said above, our measured value is an estimate of the true value.

Chapter 4 : Measurement uncertainty - Wikipedia

2. What is Uncertainty of Measurement 2 3. Reasons for Estimating Uncertainty 2 4. Sources of Uncertainty in Chemical Measurement 3 5. Evaluation Methods 4 6. Structure of Analytical Procedure 6 7. Process for Estimating Uncertainty 7 8. Reporting Uncertainty 17 9. General Remarks 18

Study outcomes The student who has successfully passed the course knows: The student who has successfully passed the course is able to: Organization of the course material The course overall volume 1 ECTS is organized in 12 sections, of which some are in turn split into smaller subsections. The following parts are found in the sections: The sections and also many subsection start with a brief introduction stating the main topic s and study outcomes of the section. The main topic of the respective section is explained in a short video lecture. The lecture is followed by a textual part. This text is in most cases meant to complement, not substitute the lecture although in some cases the contents of the lecture are also repeated in some extent. It rather gives additional explanations and addresses some additional topics that were not covered by the lecture. Most sections end with a self-test, which enables to test the acquired knowledge and skills. The tests contain questions, as well as calculation problems. On the other hand, however, they also promote thinking and provide by the feedback of the questions additional knowledge about measurement uncertainty estimation in different practical situations. So, the self-tests are an intrinsic component of the course and it is strongly recommended to take all of them. The printout of the current version of the course materials including lecture slides can be downloaded from here. Feedback is given as: Correct answer, correctly recognised and marked by the student. Correct answer, not recognised and not marked by the student. Incorrect answer, however, considered correct by the student. Explanatory feedback is displayed when wrong answer is selected. All self-tests can be taken as many times as needed and the success of taking self-tests will not influence the final grade. The participants can choose themselves how they spend their time during the course, because all graded tests are available from the beginning of the course until the end of the course. Please note, however, that the difficulty level of the tests increases as the course progresses: Because of the higher difficulty level it may be a good idea you might have to plan more time for the last weeks of the course. How much time it takes for passing the course, is very individual, but we estimate that an average participant needs h per week. Available for downloading free of charge at http: However, in the interest of better understanding and in order to stress the most important aspects of concepts, in many cases concepts are introduced by definitions that are somewhat simplified compared to the VIM. More deeply interested students are encouraged to consult the VIM. If you would like to learn more This course is part of the Excellence in Analytical Chemistry https: This course is run within the framework of the Estonian Center of Analytical Chemistry with the aim of offering easily accessible knowledge in analytical chemistry to labs and industries in Estonia and elsewhere. Main literature sources [2] This list of literature references is selecive, not exhauxtive. The references were selected based on the following criteria: These references are referred to in the course via superscript numbers in round brackets, e. Available on-line from http: Nordtest technical report , ed. Measurement Uncertainty and Statistics. Ivo teaches analytical chemistry and metrology in chemistry at all study levels and organizes short training courses for practitioners on different topics of analytical chemistry and metrology in chemistry. Lauri Jalukse, research fellow in analytical chemistry at University of Tartu. Lauri teaches analytical chemistry and metrology in chemistry at all study levels. He is continuously introducing innovative and active learning approaches into teaching. His research work is focused on metrological studies of electrochemical and optical sensors, measurements of dissolved oxygen concentration and moisture content, as well as organization of interlaboratory comparisons. Irja Helm, research fellow in analytical chemistry at University of Tartu. Irja teaches practical classes of analytical chemistry. She takes care that metrological concepts and approaches are introduced to students at as early stage of analytical chemistry studies as possible. Educational Technology Centre , University of Tartu.

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Chapter 5 : Estimation of measurement uncertainty in chemical analysis (analytical chemistry) course

Workshop on Measurement Uncertainty in Chemical Analysis Introduction The purpose of a measurement is to estimate the 'true' value of the analyte in the sample.

Chapter 6 : Measurement Uncertainty in Chemical Analysis

Measurement uncertainty a reliable concept in food analysis and for the use of recovery data? In and offlaboratory sources of uncertainty in the use of a serum standard reference material as a means of accuracy control in cholesterol determinat.

Chapter 7 : Measurement Uncertainty in Chemical Analysis - Google Books

It is now becoming recognized in the measurement community that it is as important to communicate the uncertainty related to a specific measurement as it is to report the measurement itself.