

Abstract

This chapter deals with the concept of “problem” in Analytical Chemistry, and is concerned with the impact and consequences, both internal and external, of solving analytical problems. The analytical problem as a target has invigorated Classical Analytical Chemistry with new challenges and goals beyond its chemical metrological role; also, it has led to analytical chemical knowledge crossing further traditional boundaries and reaching society at large to respond to the increasing needs for socio-economically useful answers. The ubiquity of the analytical problem in the analytical chemical and socio-economic realms has turned it into their interface and main link. So much so that solving analytical problems has become a priority goal in fulfilling the practical requirements of Analytical Chemistry; one that has required expanding the scope of representativeness to accommodate the results to the client’s requirements. This chapter describes the steps involved in the analytical problem-solving process, and the potential coincidence or divergence between the information required by the client and that actually delivered by the analytical chemist. Also, it relates “quality”, a general concept discussed at length in Chap. 8, to “analytical quality”, which constitutes the central core of the topic: solving analytical problems.

Teaching Objectives

- To introduce students to “analytical problem” and describe its elements.
- To describe the general steps of the analytical problem-solving process.
- To compare “required information” and “delivered information”.
- To emphasize the applied side of Analytical Chemistry.

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7.1 Explanation of the Slides

Slide 7.1

FOUNDATIONS OF ANALYTICAL CHEMISTRY	
PART III	
SOCIO-ECONOMIC PROJECTION OF ANALYTICAL CHEMISTRY	
	Chapter 7. Analytical problem-solving
Chapter 8. Analytical Chemistry and quality	
Chapter 9. Social responsibility of Analytical Chemistry	
PART I. INTRODUCTION TO ANALYTICAL CHEMISTRY	
PART II. THE ANALYTICAL PROCESS	
ANNEX 1. GLOSSARY OF TERMS	
ANNEX 2. ANSWERS TO THE QUESTIONS	

This slide places in Part III (Socio-economic Projection of Analytical Chemistry) and shows the other two parts of the book.

This chapter, which is the first discussing the socio-economic approach to Analytical Chemistry deployed across Part III, is concerned with solving analytical problems (that is, with fulfilling information requirements).

Slide 7.2

PART III	
SOCIO-ECONOMIC PROJECTION OF ANALYTICAL CHEMISTRY	
Chapter 7: Analytical problem-solving	
Contents	
7.1.1. Introduction to Part III	
7.1.2. Introduction to the chapter	
7.1.3. The concept of “problem” in Analytical Chemistry	
7.1.4. Integral definition of “analytical problem”	
7.1.5. Elements of an analytical problem	
7.1.6. Steps of the analytical problem-solving process	
7.1.7. Concluding remarks:	
7.1.7.1. Consistency between required and delivered information	
7.1.7.2. Analytical problem and quality	
Teaching objectives	
<ul style="list-style-type: none"> • To introduce students to the concept “analytical problem” and its elements. • To describe the general steps of the analytical problem-solving process. • To compare required information and delivered information. • To emphasize the applied side of Analytical Chemistry. 	

7.2.1. This slide outlines the contents of the chapter, which are explained in the seven sections shown. The last section comprises two sub-sections.

The chapter includes a preliminary introduction to Part III and several sections concerned with “analytical problem” and its elements. Also, it deals with the analytical problem-solving process, and relates “delivered information” to “required information”. Finally, it places the analytical problem in the context of quality.

7.2.2. At the bottom of the slide are the objectives to be fulfilled in connection with the analytical problem, the problem-solving process, and the types of information involved (required and delivered). This chapter pertains to the applied side of Analytical Chemistry.

7.1.1 Introduction to Part III (2 Slides)

Slide 7.3

Chapter 7: Analytical problem-solving

7.1.1. Introduction to Part III (I)

The topic dealt with in the last part of this book is the
SOCIO-ECONOMIC PROJECTION OF ANALYTICAL CHEMISTRY.

- ♣ The part is concerned with the **socio-economic consequences** of the results and knowledge obtained from **analytical processes** (Chapter 4), **whether quantitative** (Chapter 5) or **qualitative** (Chapter 6).
- ♣ It uses the third basic standard [(bio)chemical **information requirements** (see Slide 1.12)] to facilitate decision-making in the **social and economic realms**, and to assess to what extent such requirements are fulfilled.
- ♣ The three chapters in Part III are concerned with
 - ♦ A practical analysis of **analytical problem-solving**, that is, of the fulfilment of information requirements (Chapter 7).
 - ♦ The integral characterization of the socio-economic projection of Analytical Chemistry in the form of a **definition of analytical quality** (Chapter 8).
 - ♦ **Social responsibility** in Analytical Chemistry beyond analytical quality (Chapter 9).

7.3.1. Part III is mainly concerned with the socio-economic inputs and outputs of Analytical Chemistry.

7.3.2. The part explores the impact and socio-economic consequences of the information (results and knowledge) derived from qualitative and quantitative analytical processes. The most salient features of the analytical process, Quantitative Analysis and Qualitative Analysis are explained in Chaps. 4, 5 and 6, respectively.

7.3.3. At the heart of the part is “required information”, which constitutes the third basic standard of Analytical Chemistry. In fact, the information required by the client dictates how the analytical process is to be designed and decisions are to be made. Inevitably, such decisions have some socio-economic consequences—which also pertain to the thematic core of the part.

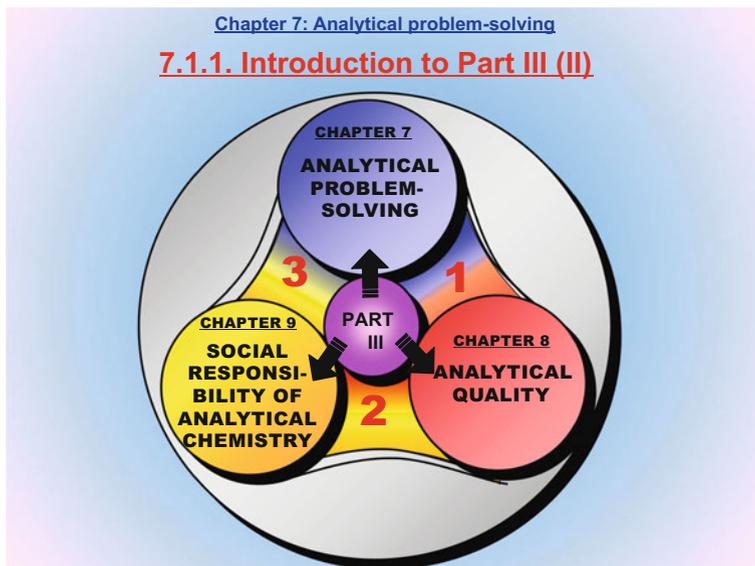
7.3.4. Part III comprises the following three chapters:

- This chapter, devoted to Analytical Problem-Solving;
- Chapter 8, concerned with Analytical Quality; and
- Chapter 9, devoted to Social Responsibility in Analytical Chemistry.

Although the socio-economic implications of Analytical Chemistry can be discussed in terms of Analytical Quality (Chap. 8), Social Responsibility (Chap. 9) constitutes the most comprehensive and faithful expression of its social and economic projection.

Despite their close relationships, the three facets are examined separately here for easier understanding.

Slide 7.4

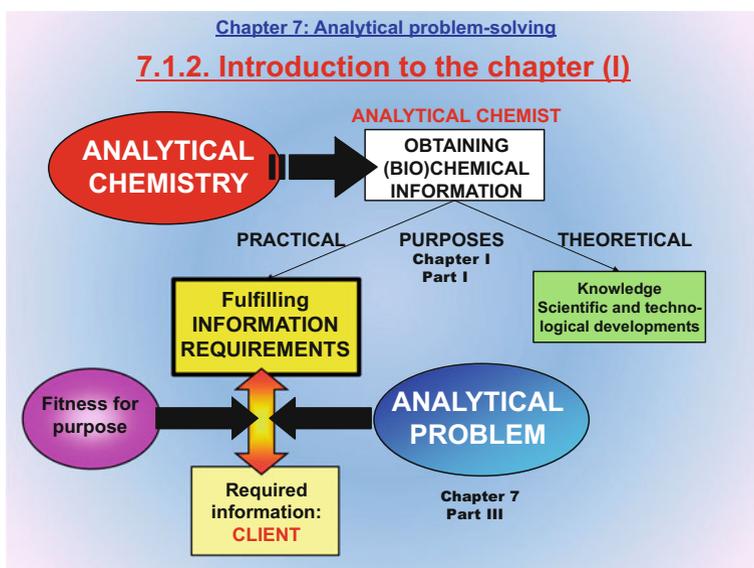


This slide connects the three chapters of Part III, which are concerned with the socio-economic projection of Analytical Chemistry. The triangle shows the three interfaces connecting the topics of this chapter and Chaps. 8, 9. As can be seen, each chapter is connected via two interfaces of the following types:

- *Interface 1.* Analytical Problem-Solving and analytical quality are related in Sect. 7.1.7.2. The basic side comprises properties or characteristics (indicators), whereas the applied side involves fulfilling information requirements (see Slide 7.28).
- *Interface 2.* Analytical Quality is only one element of Social Responsibility in Analytical Chemistry, which comprises more general social, economic and environmental implications. Even so, their internal and external connotations do not overlap in full.
- *Interface 3.* Providing a complete, honest response to specific information requirements (that is, solving the analytical problems) is the essential internal connotation of Social Responsibility in Analytical Chemistry.

7.1.2 Introduction to the Chapter (2 Slides)

Slide 7.5



7.5.1. This slide places the concept “analytical problem” in Analytical Chemistry.

As can be seen, one of the main goals of Analytical Chemistry is to obtain (bio)chemical information. The process is led and conducted by the analytical chemist.

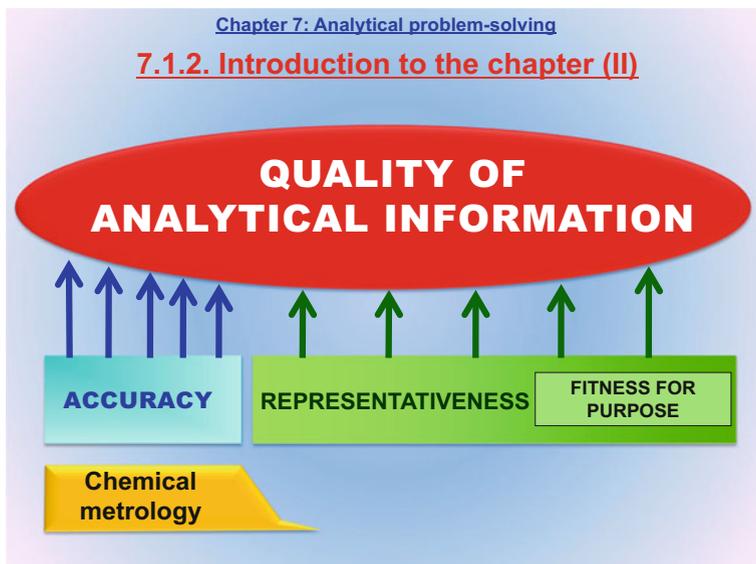
7.5.2. (Bio)chemical information can be sought for theoretical and/or practical purposes (see Slide 1.8). The practical purpose (fulfilling information requirements) is favoured over the theoretical purpose (deriving scientific and technological

knowledge, and development) here because this chapter pertains to the applied side of Analytical Chemistry.

7.5.3. The practical purpose is fulfilling a client's information requirements. Fluent communication between the client and the analytical chemist obviously requires the latter to supply the former with information that is fit for the intended purpose.

7.5.4. The analytical problem is depicted here as the interface between required information and its purpose. Fulfilling information requirements entails correctly planning and solving an analytical problem—and the problem, which is the subject matter of this chapter, connects the analytical chemist to the client.

Slide 7.6



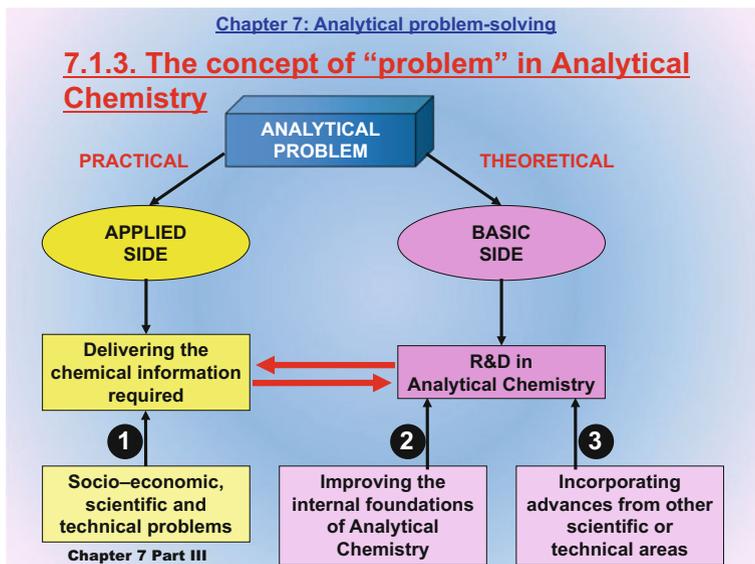
7.6.1. These are the essential ingredients of quality in analytical information, which include the capital analytical properties accuracy and representativeness (see Slides 2.4 and 2.13–2.17).

7.6.2. A third ingredient is also needed, however: fitness for purpose. This new ingredient is simply a new practical form of representativeness in Analytical Chemistry; in fact, in order to fulfil the client's information requirements (see Slide 7.5), the analytical chemist must deliver information that is fit for the intended purpose. Therefore, fitness for purpose is essential to Applied Analytical Chemistry, where it arises from the analytical problem and constitutes the third cornerstone of quality and representativeness in the results.

7.6.3. Chemical metrology is depicted here as a framework for accuracy. However, chemical metrology only includes the most orthodox notion of representativeness (namely, “internal representativeness”, Slide 7.10), without provision for “fitness for purpose” and hence for analytical problem-solving as an integral element.

7.1.3 The Concept of “Problem” in Analytical Chemistry (1 Slide)

Slide 7.7



7.7.1. The concept “analytical problem” arises on both the applied (practical) and basic (theoretical) side of Analytical Chemistry. The two sides share the goal depicted in Slide 7.5: obtaining (bio)chemical information from objects and systems.

7.7.2. On the applied side, analytical information is obtained to fulfil information requirements (that is, for the practical purpose of Slide 7.5); on the basic side, information is obtained to further knowledge, research and innovation in Analytical Chemistry (that is, for the theoretical purpose of Slide 7.5).

7.7.3. The concept “analytical problem” is connected with the basic and applied sides at points 1–3 in the slide.

- (1) On the *applied (practical) side* of Analytical Chemistry, the analytical problem arises from the need to solve social, economic, scientific and technical problems. Such problems constitute the starting point and unavoidable reference for correctly planning and solving the analytical problem. This is the facet of “analytical problem” dealt with in this chapter.
- (2) On the *basic (theoretical) side*, the analytical problem arises as an element of the internal foundations of Analytical Chemistry. In addition, the analytical problem is an incentive for improvement. Thus, solving the problem entails relying on other foundations such as *analytical properties, proper planning* and

assurance of the traceability chain, which often calls for innovation and development through research.

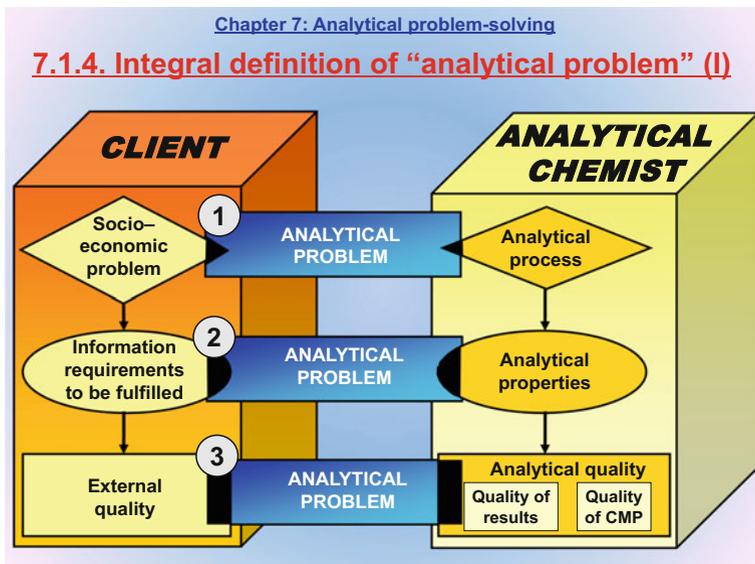
- (3) On the basic side, the analytical problem also arises as a means of connecting scientific or technical areas (that is, as a link between the shared foundations of scientific disciplines). Because the knowledge used to address an analytical problem should be consistent with the particular information requirements, Analytical Chemistry must continuously acquire knowledge and incorporate advances from different branches of science.

7.7.4. The purposes of the two sides are obviously and necessarily related by the analytical problem. Obtaining appropriate information to solve an analytical problem requires using theoretical knowledge produced by research. Also, scientific and technical research and development rest on information obtained by solving analytical problems in order to improve the theoretical knowledge base of Analytical Chemistry and propagate it to other scientific areas.

7.1.4 An Integral Definition of “Analytical Problem” (5 Slides)

The concept “analytical problem” is briefly defined and exemplified in Slides 1.28 and 1.29, respectively. This section provides a more comprehensive definition that considers its socio-economic connotations (client–chemist communication), its place in analytical concept hierarchies; its innovative, ground-breaking nature; and its traceability chains.

Slide 7.8



7.8.1. This slide deals with “analytical problem” from a socio-economic perspective (specifically, as the link between the client requiring information and the analytical chemist producing it).

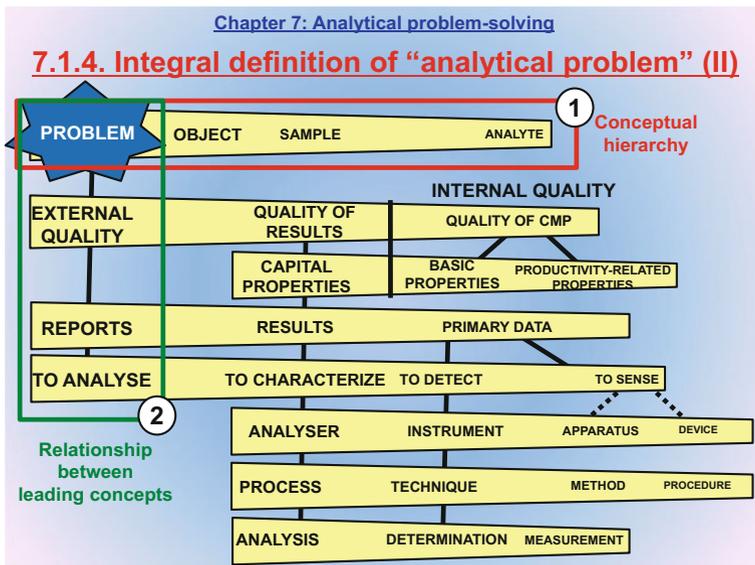
In the client’s realm fall the socio-economic problem to be solved by fulfilling specific information requirements and the external quality imposed by the client.

In the analytical chemist’s realm falls the analytical process. Depending on how effectively the process is planned and implemented, the ensuing levels of analytical properties will lead to a given degree of analytical (internal) quality (a combination of quality in the results and quality in the CMP).

7.8.2. The analytical problem arises as the interface connecting the client to the analytical chemist in three different ways.

- (1) *First*, the analytical problem is the link between the socio-economic problem on the client’s side and the analytical process on the analytical chemist’s side. Correctly planning an analytical problem in accordance with the client’s socio-economic problem entails designing a valid, assessed analytical process adjusted to the client’s information needs.
- (2) *Second*, the analytical problem connects the information requirements to be fulfilled on the client’s side to analytical properties on the analytical chemist’s side. The analytical chemist should be able to assure the levels of analytical properties required by the client; this in turn will require that the analytical problem contain any information needed to express, discard and validate the analytical properties of the associated analytical process.
- (3) *Third*, the analytical problem relates external quality on the client’s side to analytical quality on the analytical chemist’s side—a product of quality in the results and in the Chemical Measurement Process (CMP). The analytical quality arising from implementation of an analytical process should fulfil the client’s quality requirements. The analytical problem should translate external quality requirements into analytical quality goals to be reached through analytical properties of the results and the CMP.

Slide 7.9

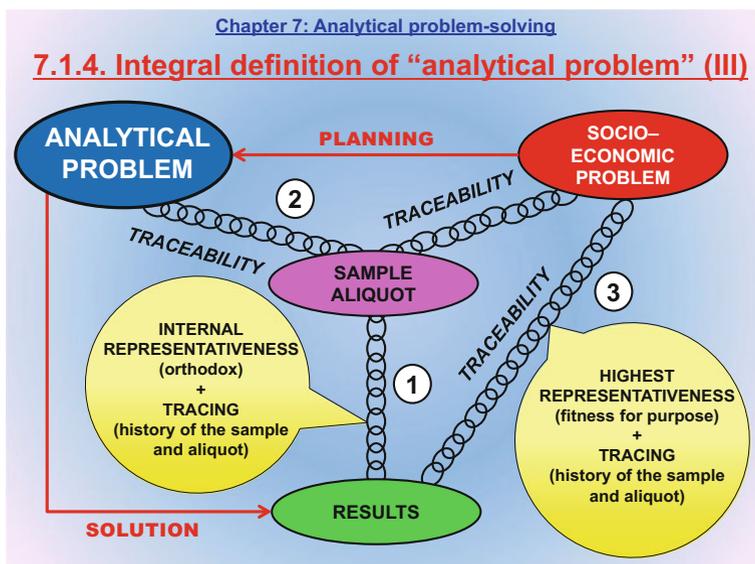


7.9.1. This slide is a conceptual and technical depiction of the hierarchies in Slides 1.21, 1.24 and 1.27. Below are discussed it most salient implications (1 and 2).

7.9.2. The analytical problem is at the top of the hierarchy and followed by “object”, “sample” and “analyte”. This ranking is further discussed in Slide 7.13.

7.9.3. The analytical problem can be related to the top concepts in other hierarchies (e.g., “external quality”, “reports” and “to analyse”). Thus, solving an analytical problem entails producing a report to compiled the information gathered and knowledge derived from results obtained by analysing. The report, which is the solution to the analytical problem, should possess internal quality (quality in analytical properties) but also external quality (the ability to solve the socio-economic problem addressed).

Slide 7.10



7.10.1. This slide shows the traceability (consistency) chains and links to be established in solving an analytical problem.

7.10.2. Link 1 is a relationship of consistency between the results and the sample aliquot—which in turn should be consistent with the sample. Assuring traceability between these two components requires that the results be representative of the assayed aliquot and the sample (internal representativeness), but also the documented history of the obtainment, processing and storage of the sample and aliquot.

7.10.3. The sample aliquot is directly connected to the socio-economic problem. It is essential that any samples collected from the object be consistent with the socio-economic problem addressed if the problem is to be correctly solved.

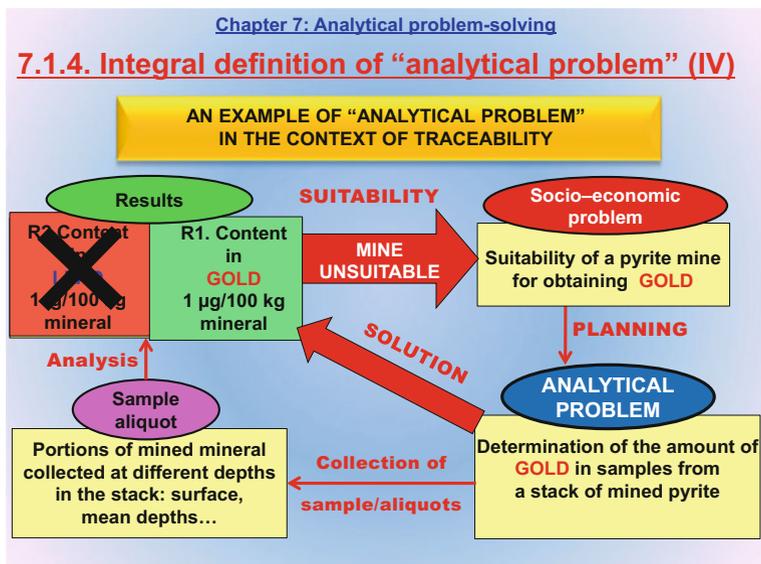
7.10.4. The analytical problem arises in adapting the socio-economic problem to the analytical chemist’s realm by adhering to the client’s information requirements. Since the analytical problem arises from the socio-economic problem, the former can be traced to the sample aliquot (2) and the chain fulfils the same representativeness and consistency conditions than that connecting the sample and its aliquot to the socio-economic problem.

7.10.5. Correctly solving the analytical problem leads to the obtainment of results that will be consistent with the socio-economic process (3). For this traceability chain to be established, the results should be accompanied by the documented history of the sample collection, processing and storage to maximize representativeness. In addition to assuring orthodox representativeness (namely, relating the results to the sample and its aliquot), maximizing representativeness

requires that the results be consistent with the information required to solve the socio-economic problem (the new ingredient of representativeness in Slide 7.6).

“Internal (orthodox) representativeness” and “maximum representativeness” (fitness for purpose) differ in that they are two facets of representativeness arising from each traceability chain. Thus, the results—sample—aliquot chain is akin to basic representativeness (a chemical metrological notion affording statistical calculation). On the other hand, the results—socio-economic problem chain rests not only on statistical representativeness but also on consistency of the results with the information requirements (that is, on fitness for purpose).

Slide 7.11



7.11.1. This slide exemplifies the traceability chains in the previous one.

The socio-economic problem addressed in the example is finding whether a stack of mined pyrite can be profitably exploited to extract gold. Pyrite is a mineral with a shiny appearance resembling that of gold.

7.11.2. The socio-economic problem here is the source of the analytical problem: assessing previously mined mineral for profitable extraction of gold. The analytical problem therefore involves quantifying the amount of gold present in a mined pyrite stack in order to find whether exploiting the stack to extract the gold would be profitable. The analytical problem is consistent with the socio-economic problem because it is its realization in the analytical chemical realm.

7.11.3. The assessment process starts with sample collection. Collected samples will be representative of the object provided they are obtained at different depths in the mineral stack in order to locate the part containing the highest concentrations of gold. Also, they will be consistent with the analytical problem and the

socio-economic problem if they are collected in accordance with the type of information to be obtained (see sampling strategies in Slide 4.16).

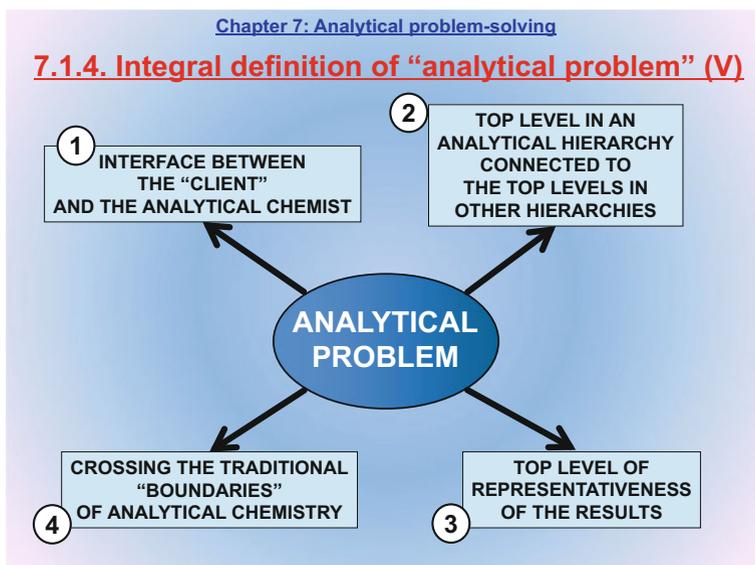
7.11.4. The analysis of each sample yields two results (outputs): the amount of gold (R1) and that of lead (R2) present in the mineral stack.

7.11.5. Only the amount of gold (R1), however, is the solution to the analytical problem here. Therefore, the other result (R2, the amount of lead) is discarded and the amount of gold (R1) is related to the analytical problem as shown in the slide.

7.11.6. After the analytical problem is solved, the true result (R1) is interpreted in order to solve the socio-economic problem. Since the amount of gold present in 100 kg of mined mineral is too small (barely 1 μg), exploiting the mine for gold would obviously be unprofitable. This information is therefore fit for the purpose and the result (the amount of gold present, R1, which is the solution to the analytical problem) is directly connected to the socio-economic problem.

A chain of three links (namely, the socio-economic problem, the analytical problem and the results) is thus established where correctly solving the analytical problem produces results that are “traceable” to the socio-economic problem.

Slide 7.12



This slide summarizes the four essential notions behind the definition of “analytical problem”.

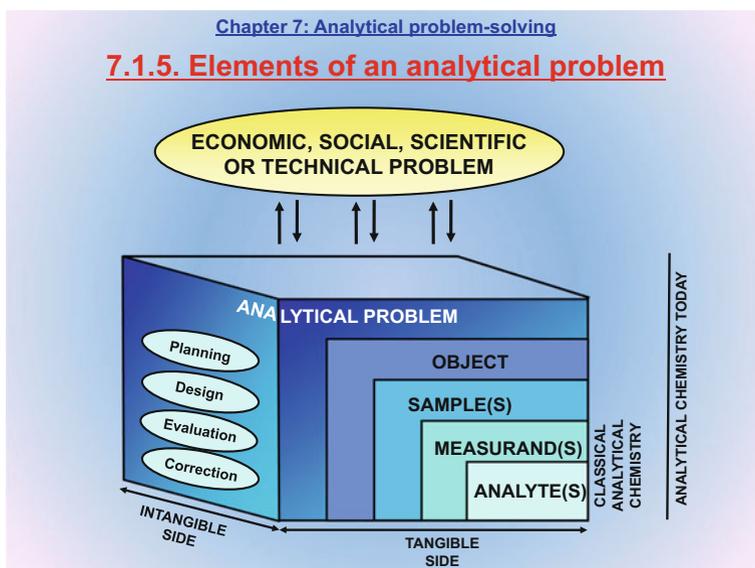
- (1) The analytical problem is the interface or link between the client and the analytical chemist (see Slide 7.8).
- (2) Also, it is the top level in an analytical hierarchy and connected to the top levels of others (see Slide 7.9).

- (3) Correctly solving the analytical problem entails maximizing representativeness in the results (that is, consistency of the results with their purpose). The concept of “maximum representativeness” in Applied Chemistry is illustrated in Slide 7.10 together with the traceability chains involving the analytical problem.
- (4) The analytical problem crosses the traditional “boundaries” of Analytical Chemistry and projects it outside the laboratory. The analytical problem as a link between the client and the analytical chemist sets a socio-economic goal for laboratory work. In this way, Analytical Chemistry acquires a new dimension in addition to its traditional function as a chemical metrological science and adopts a socially active role.

The four definitions in this slide are mutually related. Thus, the analytical problem as the interface between the client and the analytical chemist requires maximizing representativeness in order to fulfil the particular information requirements. The client–analytical chemist relation is an element of the new dimension of Analytical Chemistry (crossing traditional borders); also, it falls at the top of a hierarchy.

7.1.5 Elements of an Analytical Problem (1 Slide)

Slide 7.13



7.13.1. This slide depicts the analytical problem as a cube containing the specific information requirements of the particular social, economic, scientific or technical problem addressed. The elements of the problem are shown on two sides of the cube.

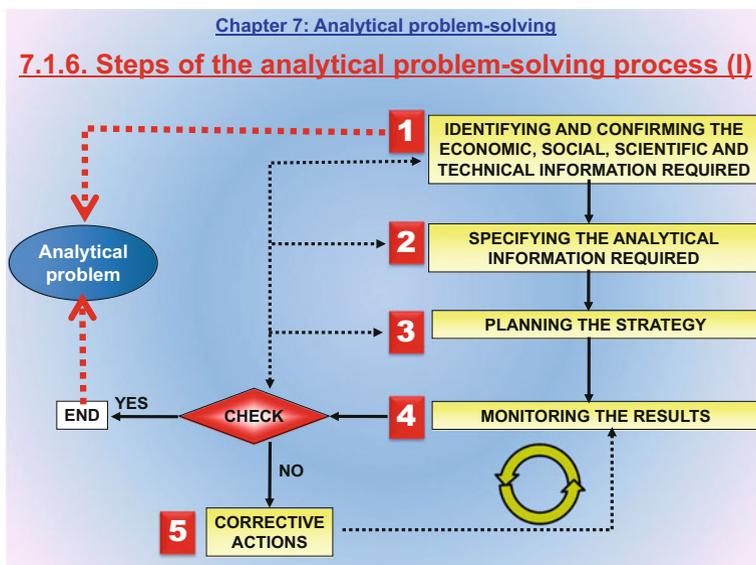
7.13.2. On the tangible side of the cube is a scope hierarchy with the analytical problem at the top. The elements of the hierarchy are defined in Slide 1.28. The object should be consistent with the analytical problem and accurately described by the results. Also, the sample should be collected in accordance with the type of information required, and the measurands and analytes should be carefully selected in order to ensure that the results can be correctly interpreted to solve the analytical problem.

7.13.3. On the intangible side of the cube are the terms “planning”, “design”, “evaluation” and “correction”, which are key actions towards solving the analytical problem. These actions are dealt with in Sect. 7.1.6.

7.13.4. The slide also illustrates the notion of “border crossing” (see Slide 7.12). Thus, incorporating the analytical problem as the realization of an actual social, economic, scientific or technical problem makes Analytical Chemistry a modern science consistent with its new goals. The analytical problem has expanded Classical Analytical Chemistry and facilitated its adjustment to the new information requirements that have emerged in recent years.

7.1.6 Steps of the Analytical Problem-Solving Process (9 Slides)

Slide 7.14



7.14.1. These are the steps to be followed in order to properly solve an analytical problem. Each individual step is described and exemplified in Slides 7.15–7.22 and briefly discussed here.

7.14.2. First step: identifying and confirming the information requirements. This entails the exchange of information between the client and the analytical chemist so that the latter can correctly plan the analytical problem to be solved in order to fulfil the information requirements of the former. This step is occasionally difficult to overcome.

7.14.3. Second step: identifying the analytical by “translating” the client’s information requirements into analytical chemical terms.

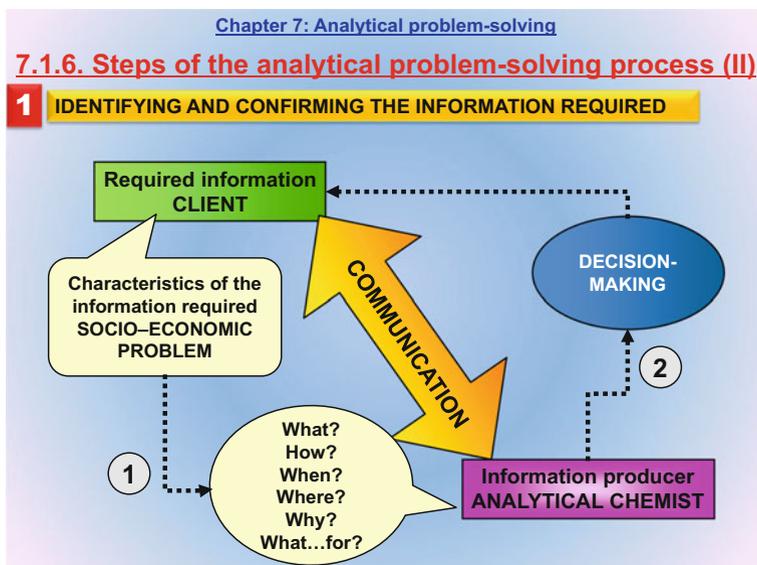
7.14.4. Third step: planning the strategy to be followed in order to obtain the information required, which roughly involves developing an appropriate Chemical Measurement Process (CMP) or choosing an existing one for the intended purpose.

7.14.5. Fourth step: monitoring the results by comparison with internal references (the analytical information required) and external references (the client’s information requirements).

7.14.6. If the results compare well with the references and are consistent with the information requirements, the analytical problem is deemed solved. Otherwise, a fifth, corrective step (7.14.7) is required.

7.14.7. Fifth step: corrective actions. Previous steps are checked in order to identify the error preventing the analytical problem from being correctly solved. Once all errors are corrected, the process returns to the fourth step (7.14.5) and the results are re-checked in order to decide whether new corrections (a new fifth stage) are needed. If none is required, the cycle is closed and the process ended.

Slide 7.15



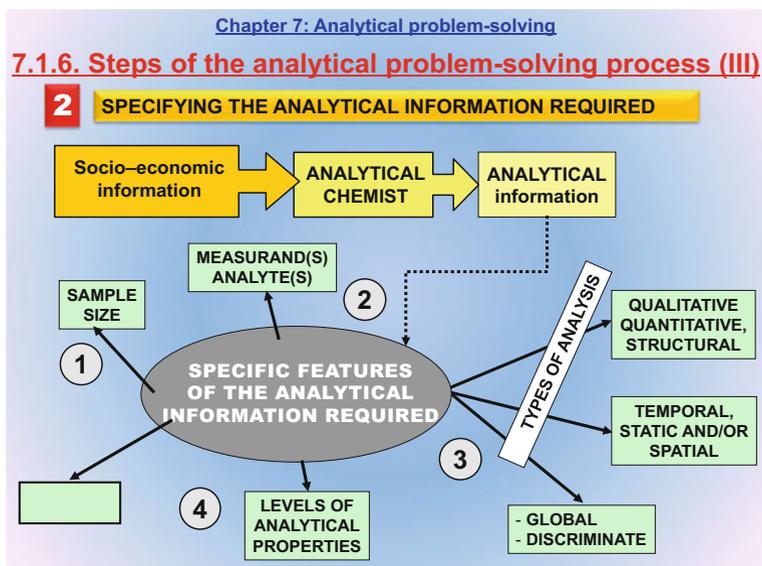
7.15.1. This slide depicts the first step of the analytical problem-solving process: identifying and confirming the information requirements.

7.15.2. Properly planning and solving an analytical problem rests heavily on accurate communication between the client and the analytical chemist so that client's socio-economic problem can be made consistent with the analytical problem to be planned and solved by the analytical chemist (that is, on assuring the traceability chain of Slide 7.10). Communication between the client and the analytical chemist should proceed via two different routes (1 and 2 in the slide).

7.15.3. Route 1. Properly planning the analytical problem requires the analytical chemist to obtain as much information about the client's socio-economic problem as possible by asking key questions such as what?, how?, when?, where?, why? or what... for?

7.15.4. Route 2. The strategy to be followed in order to solve the analytical problem depends on the particular requirements identified in this step. Such requirements provide useful clues with a view to obtaining the required information and hence facilitating decision-making by the analytical chemist. The chemist's decisions will clearly determine whether the client's socio-economic problem can be solved correctly and timely.

Slide 7.16



7.16.1. The second step in the analytical problem-solving process involves specifying the analytical information required.

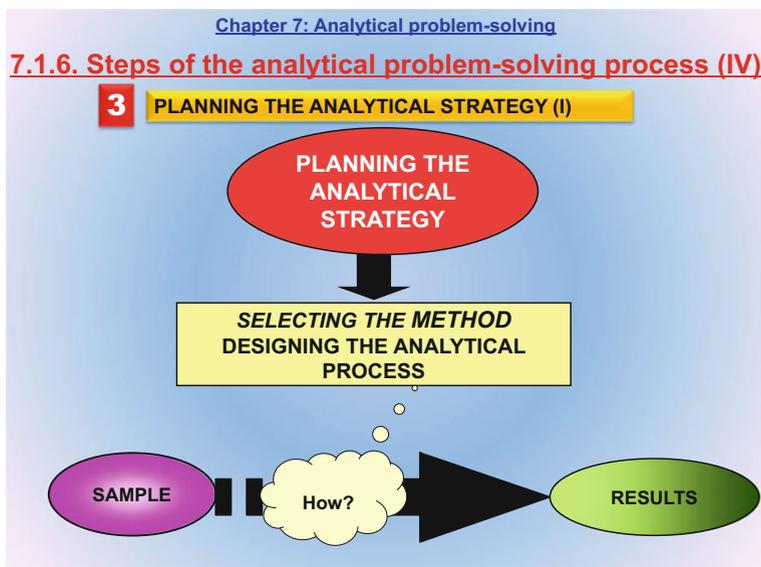
7.16.2. The client provides the analytical chemist with socio-economic information that must be translated into analytical information of use to solve the analytical problem. This is the sole responsibility of the analytical chemist, who must

establish the analytical requirements in accordance with the specific problem posed by the client.

7.16.3. The analytical information required should be carefully stated in terms such as the four depicted in the slide.

- (1) The first elements to be established are the sampling plan and the object (see sampling strategies in Slide 4.16).
- (2) Then come the measurand(s) and/or analyte(s) to be sought (that is, those to be determined in the analytical process).
- (3) Which type of analysis is to be performed comes then. The analytical chemist must choose among quantitative (Chap. 5), qualitative (Chap. 6) or structural analysis; static, temporal or spatial analysis; and global (total) or discriminate (single species) analysis.
- (4) Finally, the levels of analytical properties to be reached are established. This requires a sound knowledge of capital and basic properties in order to correctly express the results and assure the required level of confidence in them, and also of productivity-related properties in order to be able to deliver the required information in a timely manner to facilitate decision-making by the client.

Slide 7.17

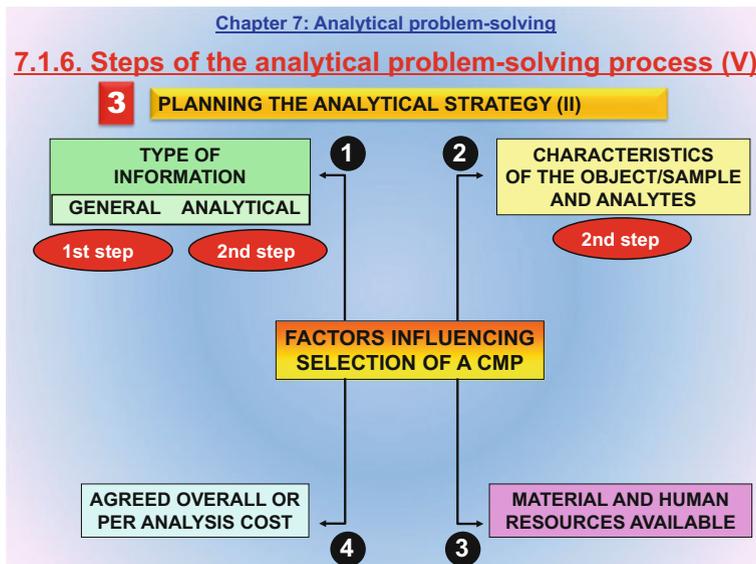


7.17.1. This is the third step in the analytical problem-solving process: planning the analytical strategy.

Planning the strategy basically entails selecting an analytical process or developing a new one for the intended purpose.

7.17.2. The aim is to answer the question “*how can the information required (results) be obtained from the sample?*” by designing an effective experimental plan.

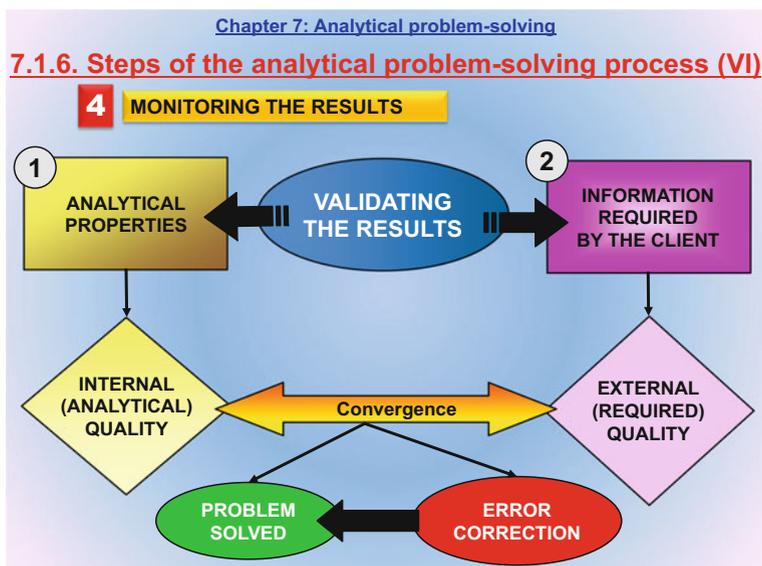
Slide 7.18



This slide shows the factors influencing selection or development of a Chemical Measurement Process (CMP) in the third step of the analytical problem-solving process.

- (1) The first factor is the type of information to be obtained (general in the first step of the process and analytical in the second). The CMP should be planned with provision for the analytical properties and type of analysis required in order to ensure that the results will be appropriate and consistent with the information requirements.
- (2) The second factor is the characteristics of the object, the sample to be analysed and the analyte to be sought or quantified. The nature of the object, sample and analyte will dictate the sampling plan, the preliminary operations to be conducted and the specific method to be used to determine the analyte. These factors are all parts of the analytical process and should therefore be considered in its development.
- (3) The third factor is the material and human resources available to the analytical chemist. Such resources include laboratory staff and equipment, which can restrict or expand the range of available analytical methods.
- (4) The last factor is the overall or individual cost agreed with the client, depending on which the range of choices may also be wider or narrower.

Slide 7.19



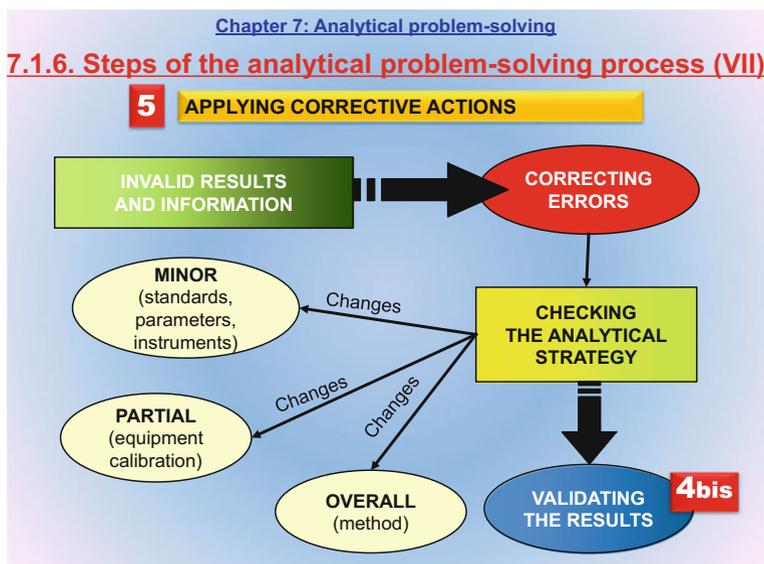
7.19.1. This is the fourth step in the analytical problem-solving process: monitoring the results by comparison with established references, which is known as “validation of the results”.

7.19.2. The process involves validating analytical properties and information as follows:

- (1) Validating the levels of analytical properties involves checking that they conform to the requirements of the laboratory (legal limit and cut-off concentration, Slide 6.13) and the client. This is the entire responsibility of the analytical chemist and assures analytical (internal) quality, which pertains exclusively to the analytical chemical realm.
- (2) Validating the information obtained against that required by the client involves checking that the results fulfil the client’s needs (i.e., that interpreting the results allows the socio-economic problem to be solved and representativeness—Slide 7.10—to be maximal as a result). At this point, the client and the analytical chemist must engage in communication as they did in the first step of the analytical problem-solving process (see Slide 7.15).

7.19.3. Validation against the two types of references allows internal and external quality to be assured. If both are adequate, their combination ensures that the analytical problem has been correctly solved. Otherwise, some error has been made in the process that will require correction so that the analytical and the socio-economic problem can be eventually solved (see Slide 7.20).

Slide 7.20



7.20.1. This is the fifth step in the analytical problem-solving process: applying corrective actions. This step is only needed when the results and information produced by the analytical chemist do not allow the analytical problem and the originating socio-economic problem to be solved. The aim is to correct errors in the process, which usually arise in the analytical strategy followed in the third step.

7.20.2. Corrective actions are performed by checking the procedures used in the process and making appropriate changes. The changes needed can be of one of the following three types:

- *Minor.* The error is easily identified and arose from a standard or an individual parameter, for example.
- *Partial.* The error is more substantial because it involves a whole instrument or its calibration, for example.
- *Overall.* The error lies in the way the procedures were developed and can only be corrected by using an alternative approach.

7.20.3. The results obtained upon correction should be validated against the references of Slide 7.19. If the new results are valid, the analytical and socio-economic problem can be deemed solved; otherwise, new corrections will be needed. The cyclic nature of the process as shown in Slide 7.14 emerges here as well: “4bis” denotes repetition of the fourth step and connects corrective actions to monitoring of the results.

Slide 7.21

Chapter 7: Analytical problem-solving

7.1.6. Steps of the analytical problem-solving process (VIII)

EXAMPLE: SOLVING A SPECIFIC ANALYTICAL PROBLEM (I)

SOCIO-ECONOMIC PROBLEM:
Rejecting (action) orange ice creams (what?) if they contain colorant E-127 (erythrosine) because it may cause thyroid disorders (why?).

1 IDENTIFYING THE INFORMATION REQUIRED:
Amount of erythrosine in orange ice creams from different manufacturers.
Highest allowed additive concentration: 1 ppm.
Best before date of the ice creams: 2 weeks.

2 SPECIFYING THE INFORMATION:
A qualitative and quantitative study of orange ice cream samples from different manufacturers (is there any erythrosine?, how much?).
Highest limit of quantitation: 1 ppm.
Expeditiousness needed.

7.21.1. This slide and the next exemplify the process used to solve a socio-economic problem by solving an analytical problem as described in Slides 7.14–7.20.

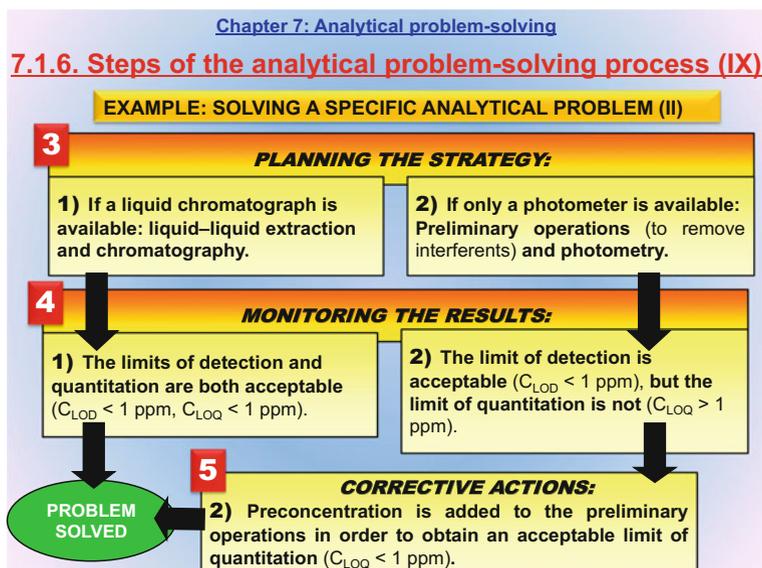
The problem in question is rejecting ice creams potentially containing a deleterious additive: the food colorant erythrosine. The information gathered from the statement of the socio-economic problems is the answer to the questions what? and why?, namely: rejecting, orange ice creams and the presence of additive E-127 (erythrosine), respectively.

7.21.2. The first step in the process involves identifying the client's information requirements. Communication between the client and the analytical chemist allows the information in box 1 to be gathered.

7.21.3. The second step involves translating the information obtained from the client into analytical information. Determining the amount of erythrosine (the client's requirement) entails previously checking that the ice creams contain it (that is, a qualitative study) and, if they do, measuring the amount present (that is, a quantitative study). Also, if the legal limit for the substance is known, the laboratory can establish a cut-off concentration such that the accepted limit of quantification will coincide with the legal limit (1 ppm). Because the ice creams have a best before date of only 2 weeks, the analytical property "expeditiousness" comes into play.

The problem-solving process is continued in the next slide.

Slide 7.22



7.22.1. The third step of the problem-solving process is approached in two different ways here, namely:

- *Strategy 1.* If a liquid chromatograph is available, the procedure of choice is liquid-liquid extraction of the additive (erythrosine) and direct determination on the chromatograph.
- *Strategy 2.* If only a photometer is available, the procedure requires some preliminary operations prior to determining the analyte photometrically.

7.22.2. The quality of the results will depend on whether strategy 1 or 2 is used.

- *Strategy 1.* The limits of detection and quantification of the chromatograph are both lower than the legal limit. As a consequence, the determination method provides acceptable levels of analytical properties and the results allow the analytical problem and the socio-economic problem to be correctly solved.
- *Strategy 2.* The limit of detection of the photometer is lower than the legal limit and hence acceptable; however, its limit of quantification is higher than the legal limit and hence useless. This entails performing some corrective action to enable the photometric determination of the colorant without interference.

7.22.3. Because the chromatograph provides valid results, the problem is solved. Thus, fifth step (corrective actions) is only needed with the photometer.

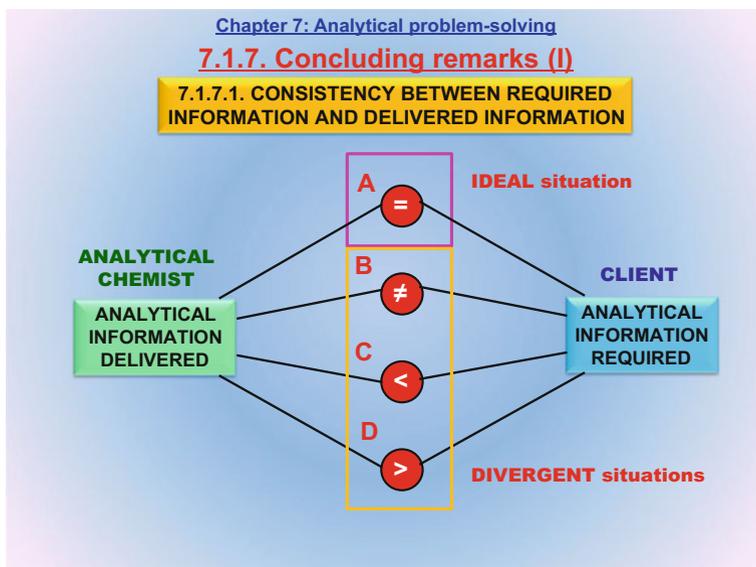
7.22.4. In *Strategy 2*, the limit of quantification of the photometric determination is improved by expanding the preliminary operations of the analytical process with a preconcentration step. This allows the analytical problem, and hence the originating socio-economic problem, to be solved.

7.1.7 Concluding Remarks (6 Slides)

7.1.7.1 Consistency Between Required Information and Delivered Information (5 Slides)

Correctly solving the analytical and socio-economic problems entails assuring that the information supplied by the analytical chemist is consistent with that required by the client. This section discusses and exemplifies various potential outcomes in comparing the information required and that actually delivered.

Slide 7.23



7.23.1. This slide depicts the four possible outcomes in comparing the information supplied by the analytical chemist and that required by the client.

7.23.2. Ideally (*situation A*), the information supplied by the analytical chemist is consistent with that required by the client (hence the = sign).

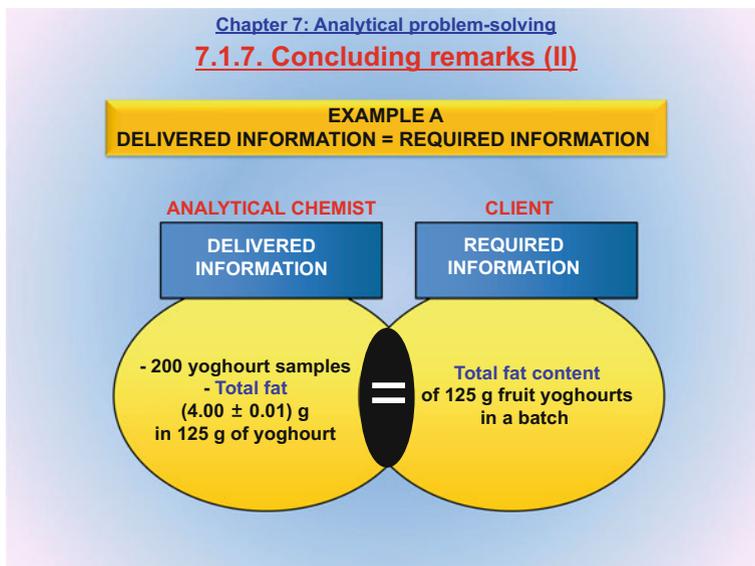
7.23.3. This is not the case with the three divergent situations denoted by letters B, C and D, and the signs \neq (different from), $<$ (less than) and $>$ (greater than), respectively. These situations arise when the analytical chemist fails to solve the client's problem owing to miscommunication or to some uncorrected error in the way the analytical problem was addressed.

- In *situation B*, the information supplied by the analytical chemist is completely different from that needed by the client to solve the socio-economic problem, so the delivered information is different from the required information.
- In *situation C*, the information supplied by the analytical chemist is inadequate to entirely fulfil the client's requirements. As a result, the delivered information is less than the required information.
- In *situation D*, the information supplied by the analytical chemist exceeds the client's requirements and answers additional questions not raised by the client. Therefore, the client is supplied with excess information and the delivered information is greater than the required information.

Fluent two-way communication between the client and the analytical chemist is paramount to ensure proper mutual understanding. In situations B and C, the client's requirements are not properly fulfilled; as a result, and the originating socio-economic problem cannot be solved. By contrast, the excess information produced in situation D does allow the problem to be solved but is obtained by incurring unnecessary expenses.

Slides 7.24–7.27 exemplify situations A–D.

Slide 7.24

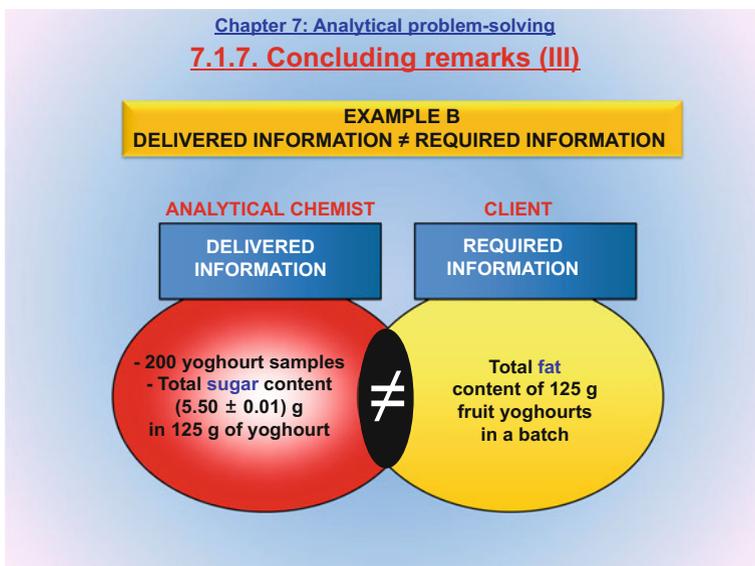


7.24.1. This slide illustrates situation A in Slide 7.23. The specific information required and that delivered are as follows:

- *Required information.* The client needs to know the overall fat content of 125 g fruit yoghourts in order to check that it meets the specifications prior to marketing.
- *Delivered information.* The analytical chemist supplies the total amount of fat in each of 200 yoghourt samples. The result is (4.00 ± 0.01) g.

7.24.2. In this situation, the information supplied by the chemist coincides (hence the = sign) with that required by the client. Communication between the client and chemist was perfect and the information requirements of the former were successfully fulfilled.

Slide 7.25



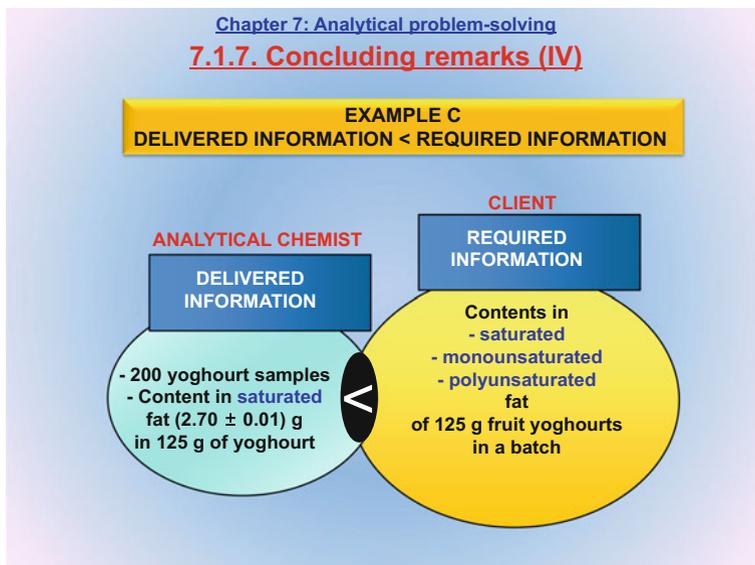
7.25.1. This slide illustrates situation B in Slide 7.23.

- *Required information.* As in situation A (Slide 7.24), the client needs to know the overall fat content of 125 g fruit yoghourts in order to check that it meets the specifications prior to marketing.
- *Delivered information.* The analytical chemist supplies the client with the total sugar content in the yoghourt as determined by analysing 200 samples. The result is (5.50 ± 0.01) g.

7.25.2. In this situation, the information supplied by the chemist is completely different (hence the \neq sign) from that required by the client, which was the fat content of the yoghourts rather than their sugar content. Communication between

the analytical chemist and the client probably failed and prevented the originating socio-economic problem from being solved.

Slide 7.26

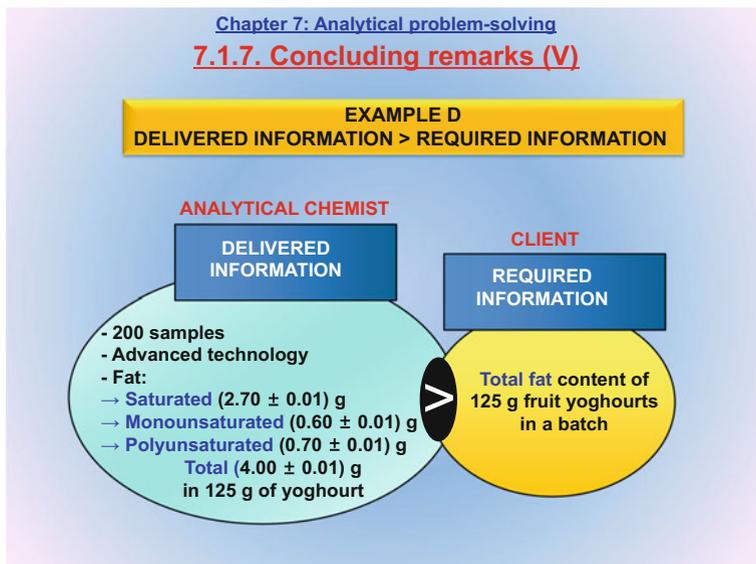


7.26.1. This slide illustrates situation C in Slide 7.23.

- *Required information.* The client needs to know the individual contents in saturated, monounsaturated and polyunsaturated fat of 125 g yoghourts in order to check that they meet the specifications prior to marketing.
- *Delivered information.* The analytical chemist supplies the amount of saturated fat in the yoghourts as determined by analysing 200 samples. The result is (2.70 ± 0.01) g.

7.26.2. The information supplied by the analytical chemist was only part (hence the < sign) of that required by the client. Communication between the two parties was probably ineffective and the client's requirements were incompletely fulfilled as a result.

Slide 7.27



7.27.1. This slide illustrates situation D in Slide 7.23.

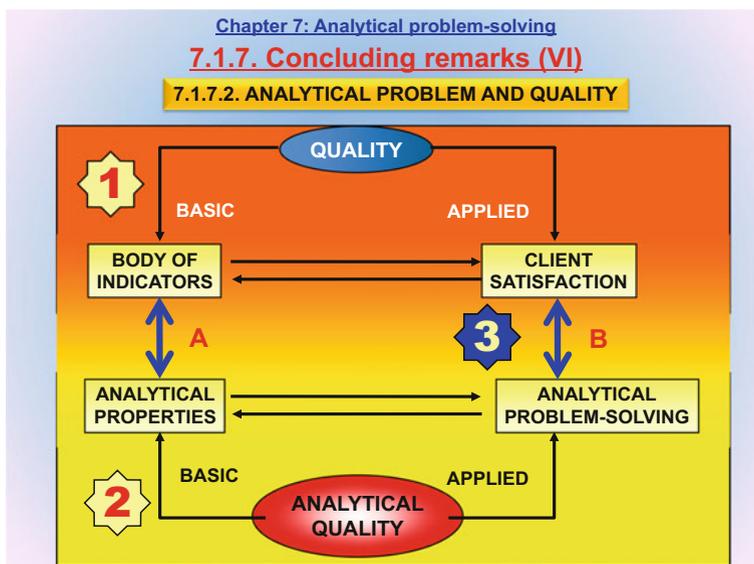
- *Required information.* As in situations A and B (Slide 7.24 and 7.25, respectively), the client needs to know the overall fat content of 125 g fruit yoghourts in order to check that it meets the specifications prior to marketing.
- *Delivered information.* The analytical chemist supplies the client with the amounts of saturated, monounsaturated and polyunsaturated fat present in the yoghourts as determined in 200 samples. The result is (2.70 ± 0.01) g for saturated fat, (0.60 ± 0.01) g for monounsaturated fat and (4.00 ± 0.01) g for polyunsaturated fat.

7.27.2. The information supplied by the analytical chemist exceeds that required by the client (hence the sign >). Communication between the two parties was successful in part. In fact, the client's information requirement was fulfilled by the analytical chemist, albeit at the expense of added costs in the additional, unnecessary determinations.

7.1.7.2 Analytical Problem and Quality (1 Slide)

Quality is the core topic in Chap. 8, which provides an integral definition of the concept (see Slide 8.5). This section deals with the concept "analytical problem" as relating to quality.

Slide 7.28



7.28.1. External (general) quality (Part 1 in the slide) can be viewed as a body of indicators (intrinsic properties inherent in external quality) and also, in practical terms, as the result of client’s satisfaction. These two views are obviously related: the body of quality indicators provides the foundation and an authoritative basis to fulfil the client’s requirements; however, satisfying the client validates the goodness (quality) of the information delivered.

7.28.2. Analytical (internal) quality (Part 2 in the slide) can be viewed as the body of capital, basic and productivity-related analytical properties (Slide 2.4), and also as the result of solving analytical problems. These two views are related as follows:

- Correctly solving an analytical problem entails assuring adequate levels of specific analytic properties in each case.
- The information and techniques used to solve an analytical problem can be incorporated into analytical chemical knowledge in order to improve analytical properties (see the relationship between intrinsic foundations in Slide 7.7).

7.28.3. Part 3 in the slide relates the general concept “quality” to the specific concept “analytical quality”. The two are related as follows:

- A. Analytical properties (Chap. 2), which are the cornerstones of analytical quality, can be used as indicators of general (external) quality. This is the

chemical metrological notion: external quality is the result of internal representativeness only (see Slides 7.6 and 7.10).

- B. As shown throughout this chapter, the analytical problem-solving process is unequivocally related to client's satisfaction. Analytical quality in the solution to an analytical problem has a direct impact on external quality because it allows a real-life socio-economic problem to be solved.

“Quality” can be defined in countless ways, but the saying “no quality is possible without a clear definition of the given task” is especially enlightening: achieving external quality from analytical quality entails solving analytical problems.

7.2 Annotated Suggested Readings

BOOKS

Principles of Analytical Chemistry

Miguel Valcárcel

Springer-Verlag, Berlin, 2000.

This was the first book to start the teaching of Analytical Chemistry with its foundations before dealing with methods and techniques in order to provide students with an accurate notion of what Analytical Chemistry is and means.

This chapter coincides largely with Chap. 7 in the book (“The Analytical Problem”). Some text in the book has been replaced with explanatory slides, however. Also, a graph depicting the traceability chains including the analytical problem has been added, and a few examples are used to illustrate traceability, the steps of the analytical problem-solving process, and consistency in the analytical chemist–client relationship.

PAPERS

The analytical problem

Miguel Valcárcel, Ángel Ríos

Trends in Analytical Chemistry, 1997, vol. 16, no. 7, 385–393.

This paper summarizes the most salient aspects of this chapter. It discusses the relationship between the analytical chemist and the client, their understanding, and the planning of analytical problem-solving processes based on their communication. Some of the slides used in this chapter originally appeared in the paper.

7.3 Questions on the Topic (Answered in Annex 2)

- 7.1. Identify the binary interfaces between Analytical Problem-Solving, Analytical Quality and Social Responsibility.

	Analytical problem-solving	Analytical quality	Social responsibility
Analytical problem-solving	×		
Analytical quality		×	
Social responsibility			×

- 7.2. What is the third basic standard in Analytical Chemistry? How is it related to the analytical problem?
- 7.3. How would you define “fitness for purpose”? To which facet of representativeness is it related? Is it related to chemical metrology?
- 7.4. Describe the roles of the analytical problem in the basic and applied sides of Analytical Chemistry.
- 7.5. How does the analytical problem relate the analytical chemist to the client?
- 7.6. What are the components of the concept hierarchy containing the analytical problem? What place does the analytical problem take in it?
- 7.7. How would you relate the analytical problem to the leading concepts “reports”, “external quality” and “to analyse” in other hierarchies?
- 7.8. Distinguish “orthodox” representativeness from “maximum” representativeness. Which traceability chain does each belong to?

- 7.9. A river is suspected to be polluted with toxic organic waste that may be having adverse effects on the nearby population. This hypothesis is verified by collecting 200 samples of water at different depths along the river for analysis. The method used has a limit of detection of 0.7 ppm and a limit of quantification of 2.1 ppm. The effects of the organic waste are felt at concentrations above 3 ppm. The concentration of waste obtained with the chosen method is 2.7 ppm. Complete the following table. Can the socio-economic problem addressed be correctly solved? Does the analytical method require any corrective actions?

Socio-economic problem	
Analytical problem	
Object	
Sample/aliquot	
Analyte(s)	
Limit of detection (C_{LOD})	
Limit of quantification (C_{LOQ})	
Legal limit (C_{LL})	
Result ($C_{obtained}$)	

- 7.10. What are the intangible elements of an analytical problem? How do they relate to the steps of the analytical problem-solving process?
- 7.11. Define and briefly describe the five steps of the analytical problem-solving process. Give an example of socio-economic problem and describe the steps needed to solve it.
- 7.12. Why is fluent communication between the analytical chemist and the client important in the first step of the analytical problem-solving process?
- 7.13. Name three essential items of information needed to identify the analytical information required in the second step of the analytical problem-solving process.
- 7.14. What is the purpose of the third step of the analytical problem-solving process? What are the factors influencing selection and design of a CMP?
- 7.15. What are the references used to assess the results in the fourth step of the analytical problem-solving process? How are they related to quality?
- 7.16. When is the fifth step of the analytical problem-solving process needed? Why?
- 7.17. How can delivered information be in relation to required information? Give an example of each situation.

- 7.18. In order to decide whether a person should be pronounced guilty of murder, a laboratory is asked to perform a comparative analysis of a blood sample from the defendant and one containing a mixture of blood from the defendant and the victim blood found in the crime scene. The analysis involves determining the DNA sequence of the defendant, the victim and the mixed blood sample. Please complete the following table by identifying the different elements.

Socio-economic problem	
Analytical problem (1st step)	
Analytical information (2nd step)	
CMP to be used (3rd step)	
Verification of the results (4th step)	

7.4 An Abridged Version of the Chapter

The contents of this chapter can be shortened for teaching Analytical Chemistry to students not majoring in Chemistry, albeit to a lesser extent than those of others because of its transversal conception. The following 7 slides (25% of all) can be omitted for this purpose:

- Section 7.1.4: Slides 7.9 and 7.13.
- Section 7.1.6: Slide 7.18.
- Section 7.1.7: Slides 7.24–7.27.