Innovating in the teaching of Chemical Equilibrium: taking effective advantage of Information and Communication Technologies

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O meu sincero OBRIGADA.

Resumo

O Equilíbrio Químico (EQ) é uma temática representativa da natureza específica da Química. A sua compreensão implica simultaneamente a conceptualização de eventos macroscópicos, explicações de carácter submicroscópico e aplicação de linguagem simbólica/matemática. O EQ é apontado como um tópico propício à utilização pedagógica das TIC (Tecnologias de Informação e Comunicação). Contudo, o crescimento do leque de recursos digitais para o ensino do EQ, verificado nas últimas décadas, não foi acompanhado de um decréscimo na sinalização de dificuldades de aprendizagem e concepções alternativas no tema. Esta constatação evidencia a importância de clarificar as circunstâncias em que os recursos digitais se revelam úteis no ensino do EQ e desenvolver módulos educativos que tenham em conta os resultados e recomendações da literatura.

Neste projecto pretende-se trazer um contributo fundamentado para o melhor aproveitamento das potencialidades das TIC no ensino do EQ. Os objectivos subjacentes a este propósito central foram delineados com base numa revisão bibliográfica que cruza três dimensões: científica, pedagógica e tecnológica. O projeto beneficiou ainda da experiência prévia do grupo no tema e da colaboração com um projecto europeu (CROSSNET).

O nível de abstração necessário para a compreensão do modelo científico do EQ é apontado como um foco de dificuldades na sua aprendizagem, sendo simultaneamente referenciado como um alvo privilegiado para intervenção das TIC. É neste contexto que o grupo introduz a expressão “facilitar a abstração”, com o sentido de auxiliar o processo de pensamento abstracto dos alunos. Esta ideia foi ganhando relevo ao longo do projecto e materializou-se no desenvolvimento de uma abordagem pedagógica com vista a facilitar a abstracção na aprendizagem do EQ. De salientar que não se pretende a criação de novos recursos digitais, numa área já saturada. A inovação reside no facto destes recursos serem englobados numa abordagem devidamente planificada e orientada para a promoção da “abstracção facilitada”.

Num modelo de investigação concebido em parceria com o projeto CROSSNET, seguiu-se a condução de um estudo de caso para obter informações sobre o funcionamento da abordagem em contexto de sala de aula, as suas mais-valias e as dificuldades associadas. Com base nos resultados obtidos foi estabelecida uma lista de recomendações, reunidos dados para a reformulação dos recursos e levantadas hipóteses para estudos subsequentes. O produto material do projecto é a abordagem pedagógica construída, a qual é disponibilizada *online*, em português e inglês, em plataformas educativas Web 2.0.

Palavras-chave: Equilíbrio Químico, abstração facilitada, recursos digitais, dificuldades de aprendizagem / conceções alternativas, módulos educativos, estudo de caso, projeto CROSSNET.

Abstract

Chemical Equilibrium (CE) is a good example of the specific nature of chemistry. The understanding of this theme requires the conceptualization of macroscopic events, as well as explanations of sub microscopic nature, application of symbolic language and mathematics. CE is commonly identified as a topic suitable for the pedagogical use of Information and Communication Technologies (ICT). However, the growth in the roll of digital resources for the teaching of CE, that took place in the last decades, was not accompanied by a decrease in the signalling of students' difficulties and misconceptions in the subject. This fact, points out the relevance of clarifying the circumstances under which digital resources turn out to be useful in the teaching of CE and develop educative modules that take into account the findings and recommendations from the literature.

This project aims to bring a contribution to take advantage form ICT potential in the teaching of CE. The objectives underlying the main purpose of the project were defined according to literature review, which crosses three fundamental dimensions (scientific, pedagogical and technological). The project also benefited from the previous experience of the group and the collaboration with an European project (CROSSNET).

The level of abstraction necessary for the understanding of the scientific model is pointed out as the major source of difficulties in the learning of CE, while also referred as a privileged target for the intervention of ICT. In this context, we introduce the expression "facilitating abstraction" to summarize the idea of supporting students' abstract thinking process during the learning of formal concepts. This idea has gained importance throughout the project leading to the development of a pedagogical approach to facilitate abstraction in the learning of CE. Although based on the use of ICT, the main purpose wasn't to introduce new digital resources in the saturated field of CE. Instead, the innovation resides in applying those resources in a properly planned approach, centred in promoting "facilitated abstraction".

The research model was designed in partnership with the CROSSNET project, consisting of the conduction of a case study for gathering information on the operation of the approach in classroom context (the major advantages, difficulties associated…) Based on the results, a list of recommendations was established, as well as indicators for the upgrade of the resources used. Some hypotheses for further studies were also raised. The ultimate product of the project is the pedagogical approach that we refer to as "FACE" -

Facilitating Abstraction in Chemical Equilibrium (learning), available online in Portuguese /English, uploaded on educational platforms based on Web 2.0.

Keywords: Chemical Equilibrium, facilitated abstraction, digital resources, learning difficulties/ misconceptions, educational modules, case study, CROSSNET project.

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Acronyms

CE – Chemical Equilibrium

CROSSNET – Crossing Boundaries in Science Teacher Education (European project)

FACE – Facilitating Abstraction in Chemical Equilibrium

FASE – Facilitating Abstraction in Science Education

ICT – Information and Communication Technologies

LCP - Le Chatelier's principle

SMR - Submicroscopic representations

STS - Science Technology and Society

Chapter 1 - Introducing the Project

1.1. Discussing the relevance and innovation of the project

This project was originated by the idea of bringing a pertinent contribution to the teaching of Chemical Equilibrium (CE) - taking advantage from ICT potential.

From background work, we have verified that Chemical Equilibrium:

- is representative of the specific nature of chemistry since it involves knowledge of macroscopic, microscopic and symbolic/mathematical nature;
- has a long tradition in learning difficulties and misconceptions, that have persisted until nowadays;
- is proposed for the use of ICT in several references from literature;
- has a large number of digital resources dedicated to its teaching, many of them available online.

Studies in chemistry education, published in recent decades, point to the relevance of digital resources in the learning of this and other such issues, dependent on microscopic models and abstraction abilities. The evolution of computers multiplied the creation of digital resources for the teaching of CE that are now spread throughout the Web, particularly animations and computational simulations. However, the wide availability of online resources for this theme contrasts with the persistence of numerous learning difficulties and misconceptions, identified in the literature. This contradiction highlights the need to develop studies in order to understand the circumstances that enable ICT's potential to the teaching of CE. This context also reminds us of the importance of developing educational modules that take into account the results and recommendations from literature. These findings, combined with the representative nature of CE, show the relevance of using this subject as a base for research on the potential of ICT for chemistry education.

Creating new digital resources was never planned as the main purpose of this project, since CE is an area saturated with educational products based on ICT, several of them available *online*. Indeed, a computational simulation, which resulted from previous work of the group, was already available for the project. Instead, our main purpose was to contribute to the clarification of the conditions under which digital resources can be useful in the teaching of CE. In order to achieve this goal, we considered the specific demands of the subject and the findings and recommendations from literature on the development of an approach carefully planned to take advantage from ICT in the teaching of CE.

The above paragraphs show that this project congregates three main dimensions: scientific (chemistry), technological (ICT) and pedagogical (Chemical Equilibrium teaching/learning), which are the object of the literature review presented in the next chapters.

Chemistry is simultaneously the starting and the ending point, since the focus resides in a subject from the chemistry curriculum: Chemical Equilibrium. On chapter 2 we reflect on the particularities of this science and analyse the subtleties of the Chemical Equilibrium concept.

Chapter 3 is centred in the pedagogical dimension, focusing on learning theories. Cross-referencing scientific and pedagogical dimensions, at the end of Chapter 3, we intend to identify the motives for the difficulties in the learning of CE and theorize about strategies to minimize them.

On chapter 4, we move on to the technological dimension, presenting, some of the possibilities opened by ICT. We briefly discuss the potential of digital resources in education, reflecting on the past, analysing the present and theorizing about the future. Also, we select the more promising features of digital resources that can be applied in the teaching of CE model. Finally, on the intersection of three dimensions we develop an approach for the teaching of CE, relying heavily on a planned use of digital resources.

Summarizing, this project strives to contribute for a better use of ICT's potential in the teaching of Chemical Equilibrium, by the identification of factors that determine the effectiveness in this area as well as the definition of strategies that lead to enhancements in the process. The scheme of Figure 1.1 summarizes the above exposed reasoning.

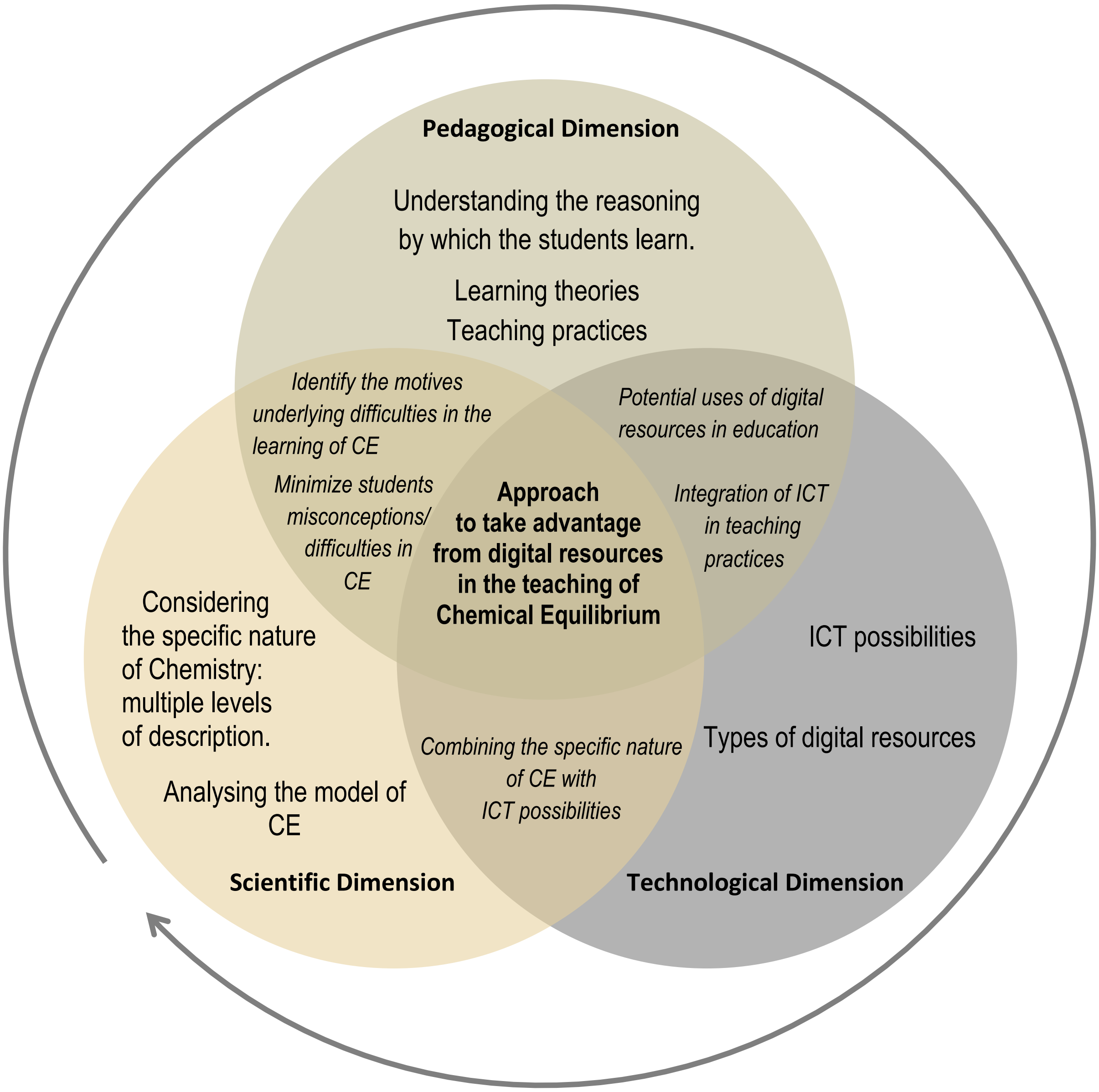


Figure 1-1 Project dimensions and the outcomes of their intersection

Throughout this investigation, facilitating abstraction in CE learning was an idea that gained importance, since the indicators from literature “blame” the abstraction level necessary to understand CE as a major source of difficulties, but also as target to apply ICT’s capabilities. So, it started to become clear that one important way to take advantage from ICT in the teaching of CE was to make it easier for the students to reach the abstraction level necessary to understand CE concepts. Note that we do not intend to lower the level of abstraction that a student needs to achieve. Instead, we intend to reach the same level of abstraction through an “aided” process, favouring the chances of success in the understanding of the same concepts.

Figure 1.2 summarizes the context that brought about the idea of “facilitated abstraction”. Since Chemical Equilibrium’s model is based on formal concepts, students’ abstraction abilities are frequently not developed enough to allow the adequate understanding of this concept. In this way, misconceptions and learning difficulties tend to arise. The representation and visualization potential of digital resources can be used to support the abstraction process, favouring the achievement of the level of abstraction that understanding CE requires. These digital resources need to be used as part of planned strategy, where the teacher plays an essential part. Studying the key features to include in this strategy, that we named FACE (Facilitating Abstraction in Chemical Equilibrium), is one of the main purposes of this project. In the context of this project FACE approach is developed in the framework of the chemistry curriculum for high school.

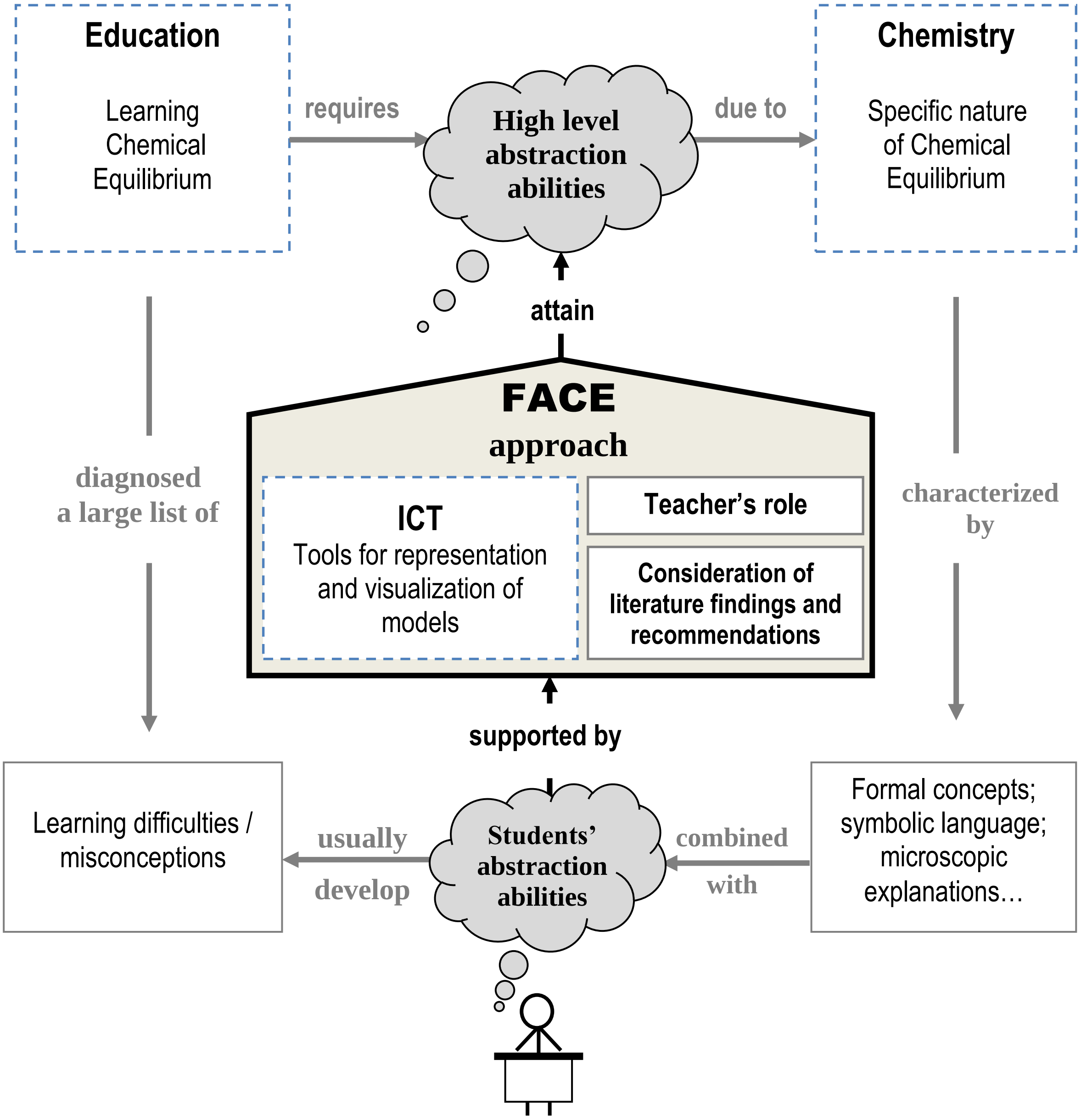


Figure 1-2 – The context for the development of FACE approach.

The fact that the idea of facilitating abstraction was growing during the project led to a gradually deeper interest in the "meanings" of abstraction and its importance for learning. This, combined with the fact that ICT in education is a constantly evolving field, explains the need we felt to revisit literature review in later stages of the project, justifying the reference of some recent works in next chapters.

Throughout the thesis, when we refer to FACE we mean facilitating abstraction in Chemical Equilibrium learning. So, although we work on a teaching strategy, it is the students' abstract thinking that we intend to support through our pedagogical approach, thus explaining the reference to the learning (not to the teaching) when speaking about facilitating abstraction.

The main innovation associated with the project resides in planning the use of digital resources to facilitate the abstraction process necessary to understand CE. The design of this approach is grounded on information from literature review presented along the next chapters, namely studies concerning the specific nature of chemistry and CE, difficulties found in the teaching of CE and research on the use of ICT in Education. Thus, the materials are screened, adapted and organized in a strategy that takes into account research results in order to "harness" the ICT potential for the teaching of CE. Later, the approach is applied on the classroom, in order to understand how the theoretical assumptions, used for its' design, work in the real context.

One important feature of this project is that digital resources constitute a means to attain a pre-defined pedagogical purpose. This kind of studies, in which carefully designed multimedia are properly embedded in an overall teaching approach, are referred as a potentially fruitful course for chemistry education research in the near future (de Jong & Taber, 2014). Several important studies from literature (that will be referred in next chapters) were focused in a more general intention of deciding whether a certain digital resource revealed itself useful in science teaching. In our case, the resources are part of a plan previously delineated and the main focus does not reside in evaluating whether an ICT based strategy is useful in bringing improvements in learning, measuring the gains quantitatively. In this case we are mostly interested in finding how an ICT based strategy can be useful in the teaching of Chemical Equilibrium while understanding the circumstances that facilitate abstraction in the learning of this theme. This will be exposed in the methodology overviews in section 1.4. We intend to shine a light over preponderant factors for taking advantage from ICT in the teaching of CE.

From the conclusion of this work two different types of results arise. The practical outcome is FACE (Facilitating Abstraction in Chemical Equilibrium): a strategy, based on

ICT, planned in order to facilitate abstraction in the learning of CE. The second outcome is more conceptual in nature: a list of recommendations to facilitate students' abstract thinking during the teaching of formal concepts. This outcome can be the basis to design similar strategies, extending the concept to other subjects (FASE -Facilitating Abstraction in Science Education).

1.2. Background work / partnerships

The inspiration for the theme and the initial phases of this project came from:

- the previous experience of the group, including a master degree about subtleties of the concept of CE and the use of computational simulations in the teaching of this subject (Fonseca, 2006);

- the partnership with European project CROSSNET (Paiva & Fonseca, 2012).

The work on the above referred master's degree was conducted according to the following stages:

- Literature review about the teaching of CE: scientific models used, pedagogical approaches and key difficulties identified in the learning process;

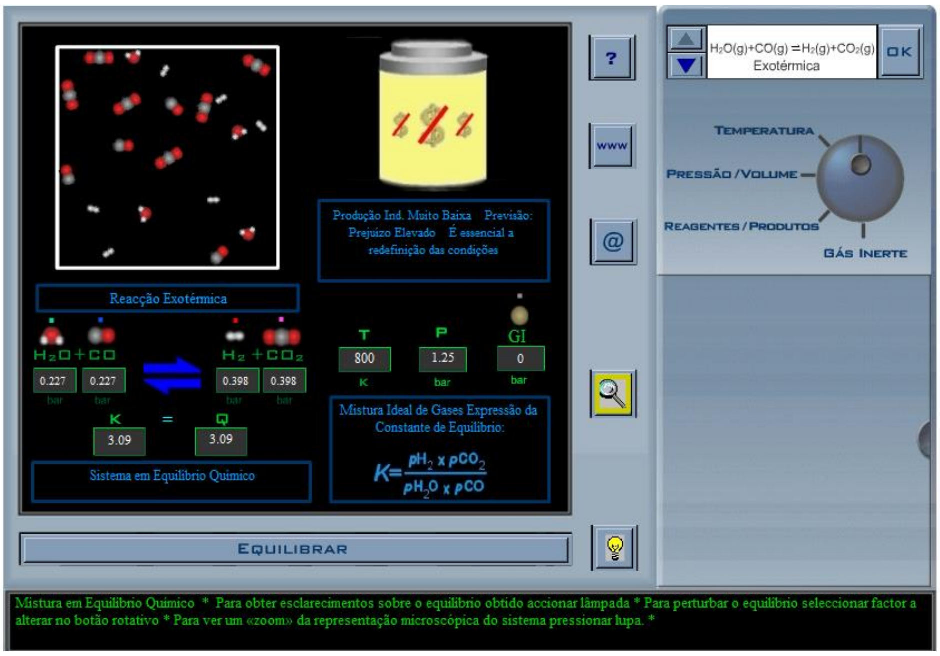
- Clarification of the scientific approximations used when explaining the influence of inert gases in chemical equilibrium state. This study indicates that inert gases have an effect over real systems in chemical equilibrium (Paiva et al., 2008). The effect is only negligible in ideal systems, showing that the usual explanation given when teaching inert gases perturbation to chemical equilibrium consists in an approximation (Paiva et al., 2008);

- Description of the "state of art" related to computational simulations available online for the teaching of Chemical Equilibrium;

- Construction of a prototype simulation, first publicized at national level in Portuguese (Fonseca et al., 2005), able to introduce improvements in this area, namely the more realistic behaviour of the system under influence of inert gases;

- Preliminary study of the impact of the prototype, with the collaboration of chemistry teachers that explored the simulation.

Teachers recognized pedagogical relevance in the simulation, characterizing it as a motivating strategy and “facilitator of learning”. At the time of this dissertation, some purposes for the future were drawn: the prototype reformulation, possible support materials...



$H_2O(g)+CO(g)=H_2(g)+CO_2(g)$
Exotérmica

Produção Ind. Muito Baixa Previsão: Prejuízo Elevado É essencial a redefinição das condições

Reacção Exotérmica

$H_2O + CO$ ⇄ $H_2 + CO_2$

H_2O	CO	H_2	CO_2
0.227 bar	0.227 bar	0.398 bar	0.398 bar

K = Q
3.09 = 3.09

Sistema em Equilíbrio Químico

T	P	GI
800 K	1.25 bar	0 bar

Mistura Ideal de Gases Expressão da Constante de Equilíbrio:

$$K=\frac{pH_2 \times pCO_2}{pH_2O \times pCO}$$

Mistura em Equilíbrio Químico * Para obter esclarecimentos sobre o equilíbrio obtido accionar lâmpada * Para perturbar o equilíbrio seleccionar factor a alterar no botão rotativo * Para ver um «zoom» da representação microscópica do sistema pressionar lupa. *

Figure 1-3 Prototype of a computational simulation for the teaching of Chemical equilibrium (Fonseca, 2006).

After this work was finished, the digital resource available for the group had its’ value recognized by an external group of teachers, while still in a phase of prototype. This stage is propitious to the use in further studies in order to clarify its potential and gather information for reformulation/upgrade. Also, the group was conscious of the state of art in the teaching of CE: “…several publications show the importance of using ICT in teaching Chemical Equilibrium. In fact, a considerable amount of resources are available online for teaching this theme, nevertheless we continue to see reports of difficulties and misconceptions. This scenario should stress the importance of carefully planning the design and use of ICT approaches, taking under consideration points like the conclusions from previous studies, the relevance of the materials involved and the role of the teacher" (Paiva & Fonseca, 2012). It was in this context that the opportunity to cooperate in CROSSNET project appeared.

CROSSNET was an European project centred in "crossing boundaries" in science teacher education (Olson & Hansen, 2012) within the EU. According to Tuomi-Grohn and Engeström (2003) "crossing boundaries involves encountering difference, entering into territory in which we are unfamiliar and, to some significant extent therefore, unqualified". Lang (2007) writes about the meaning of the term in the context of CROSSNET: "boundaries to be crossed can be identified between subjects in the sciences, mathematics or languages, between in-service teachers, between initial and in-service teachers, between theory and practice, between, and inside case study schools and between schools, university, museums, companies, plants and a number of key policymakers and stakeholders".

Each participating country (Germany, Austria, Denmark, Spain, Ireland, Poland and Portugal) has developed an innovative project, with subsequent implementation of a case study for the analysis of the events and phenomena involved. We have designed the Portuguese contribution for this European project (Fonseca & Paiva, 2006) by combining CROSSNET's focus on boundary crossing with our own background work. From Lang's (2007) description, we can situate our main field of interest in the boundaries between theory and practice, namely the barriers faced when transferring research results on the use of ICT and learning difficulties into teachers' practice in the classroom: "we identify boundaries between teaching theories/teacher education and effective classroom practice. Crossing these boundaries implies overcoming barriers between theory and practice, which arise while applying knowledge acquired during their training period in the teachers' professional daily work. Communication among teachers and with teacher educators, university professionals and other actors in education also becomes important at this level." (Paiva & Fonseca, 2012).

Based on these ideas, our contribution to "boundary crossing" consisted in the development of strategies for overcoming obstacles/difficulties found in the teaching/learning of Chemical Equilibrium through the use of ICT (Paiva & Fonseca, 2012). The name of the Portuguese contribution to CROSSNET, "EquilibrAction", was selected by associating "equilibrium" with "action", symbolizing the intention to promote innovative actions in the teaching/learning of Chemical Equilibrium.

The specific boundaries to work on, were defined by combining references about learning difficulties in CE, valued teaching methodologies and the use of computers in education, and can be expressed as the switch from:

- passive learning to active learning;
- learning the concepts to learning in context;
- formal abstraction to facilitated abstraction.

Crossing these boundaries implies distancing ourselves from traditional methods in the teaching of CE and approaching territories commonly unfamiliar to teachers and students, meeting Tuomi-Grohn and Engeström's definition (Tuomi-Grohn & Engeström, 2003).

A case study was conducted around each of the "pairs" referred above, where the conditions for / implications from transposing these boundaries were analysed. At the students' level the analysis consisted of the improvements/changes on learning and at the teachers' level it was based on the reflections about moving from the theoretical background to the effective classroom performance (Paiva & Fonseca, 2012). Another central purpose of the project was the development of innovative approaches, in cooperation with chemistry teachers. These approaches constitute a strategy that integrates a central resource supported by several materials. Their design was based on indicatiors from previous studies, in order to favour the integration of theory into practice.

From the already reported background of the group, our participation in CROSSNET had a direct focus on the improvement of students' learning of CE. Nevertheless, remembering that CROSSENT revolved around "science teacher education", the concretization of the Portuguese proposal was also intended to promote innovation of pedagogical practices and the teachers' professional development (Paiva & Fonseca, 2012). The Portuguese collaboration in CROSSNET was not directly focused in a program for teacher education, assuming a more modest contribution at this level than the work done in other countries. Nevertheless, the work on CROSSNET's Portuguese cases promotes change in the practices of the teachers involved and implies crossing boundaries between teaching theories and classroom practice. The student may be the final target of our contribution, but to the teacher belongs the leading role of triggering the change that ultimately benefits the student. This is again according to the theoretical background on boundary crossing: “in the face of such obstacles, boundary crossing seems to require significant cognitive retooling” (Tuomi-Grohn & Engeström, 2003). Each case study included a reflexive dimension about the implications from the use of these approaches in teachers’ pedagogical practice.

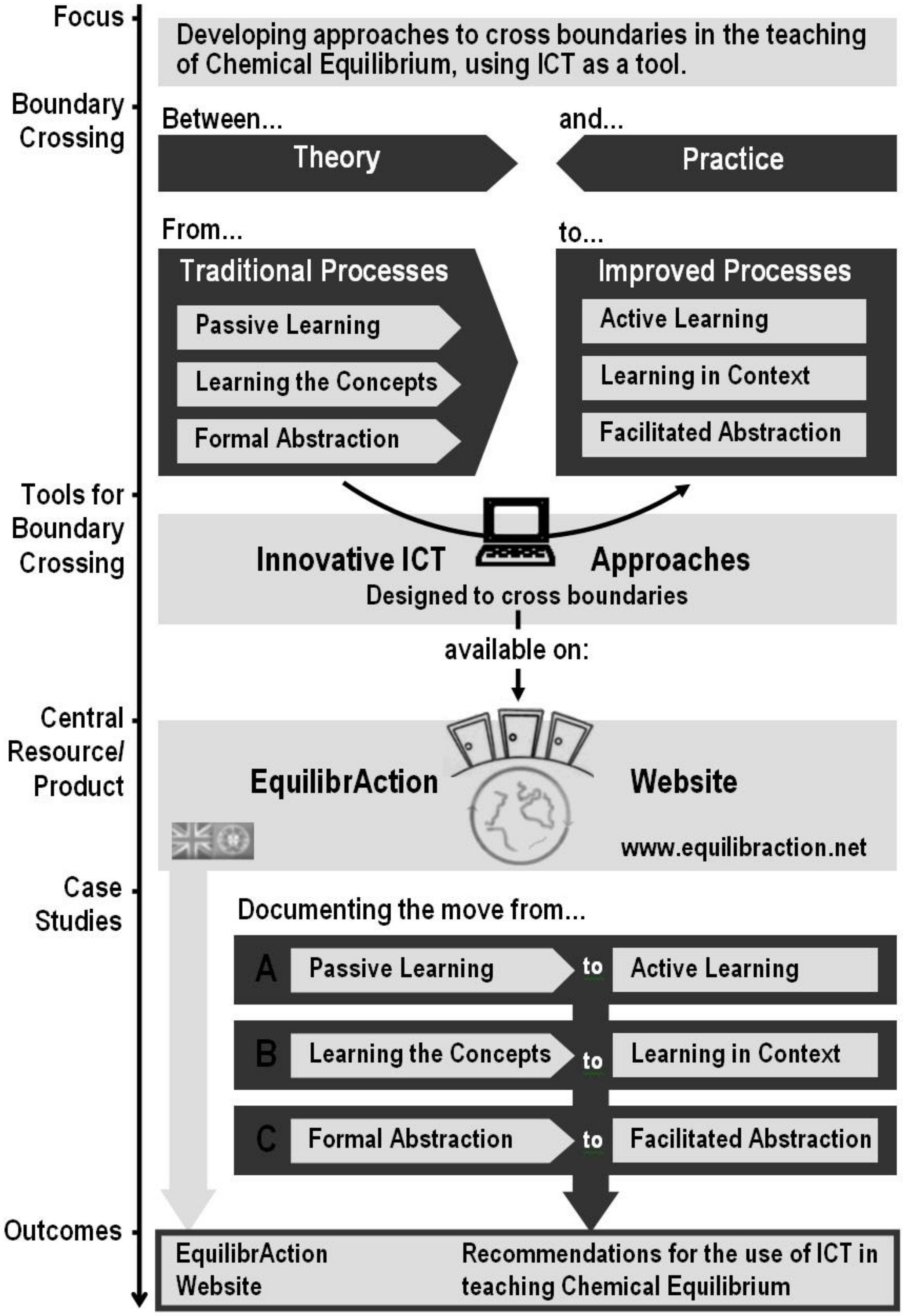


Figure 1-4 Portuguese participation in CROSSNET (after Paiva e Fonseca, 2012).

During the project, we studied the conditions for and the implications of crossing boundaries. The first pair (passive learning/active learning) focuses in improving the student’s participation in learning processes. The second pair (learning the concepts/learning in context) refers to a situation in which the student learns the theme integrated in related contexts, by associating the concepts with daily or technological issues. Finally, in the last pair (formal abstraction / facilitated abstraction) it is intended to facilitate the process of abstraction, usually formal, using appropriated teaching approaches.

Settling synergies between this PhD project and the participation in CROSSNET allowed to benefit from group dynamics, exchange of ideas and experiences for the refinement of the work. As a result, the work on the boundary between “formal abstraction” and “facilitated abstraction” began in a CROSSNET context and was then extended into this PhD project. As pointed in section 1.1, it was found that the Chemical Equilibrium is a formal concept that implies abstraction capacity for its understanding. It was, thus, clear that the abstraction effort required to understand the concepts is one of the barriers to work on the teaching of Chemical Equilibrium. Because of this, we introduced the term "facilitating abstraction" to the desired learning environment supported by the representative capabilities of the computers.

Summarising, in CROSSNET the "facilitated abstraction" was one of the barriers in study, along with the other two. An integration of the results from three case studies was made, in order to toughen the investigation and establish a more general guidance on the use of computers in the teaching of CE. During the development of the project, case studies were conducted by the teachers, each referring to the application of one of the approaches inside the classroom and using different instruments for data collection. From a cross analysis of the embedded cases, the conclusions of the national case were drawn. Indicators show the ICT approaches as being positive contributions under the conditions established. One of the outcomes of this work is a list of recommendations concerning the use of ICT in teaching Chemical Equilibrium, which highlight the relevance of using appropriate support materials and the importance of predicting/identifying possible barriers. The results from the work in CROSSNET will be exposed in more detail in chapter 7.

During CROSSNET, the group used a Website, whose development was planned after CROSSNET for organizing the resources in a portal about Chemical Equilibrium. Nevertheless, the evolution in informal ways of learning, with the emergence of Web 2.0 led the group to abandon the idea of an exhaustive portal and embrace the upload of the material in web 2.0 based portals, directed to science teachers' communities. This option will be discussed in later chapters.

Summarizing, this partnership has several contributes to the present dissertation:

- it allowed the exchange of knowledge internationally;
- directed the investigation to the conduction of a case study;
- focused the group in the framework of transposing boundaries, in a sense of overcoming obstacles, which drew attention later to overcoming the abstraction barrier in the teaching of CE.

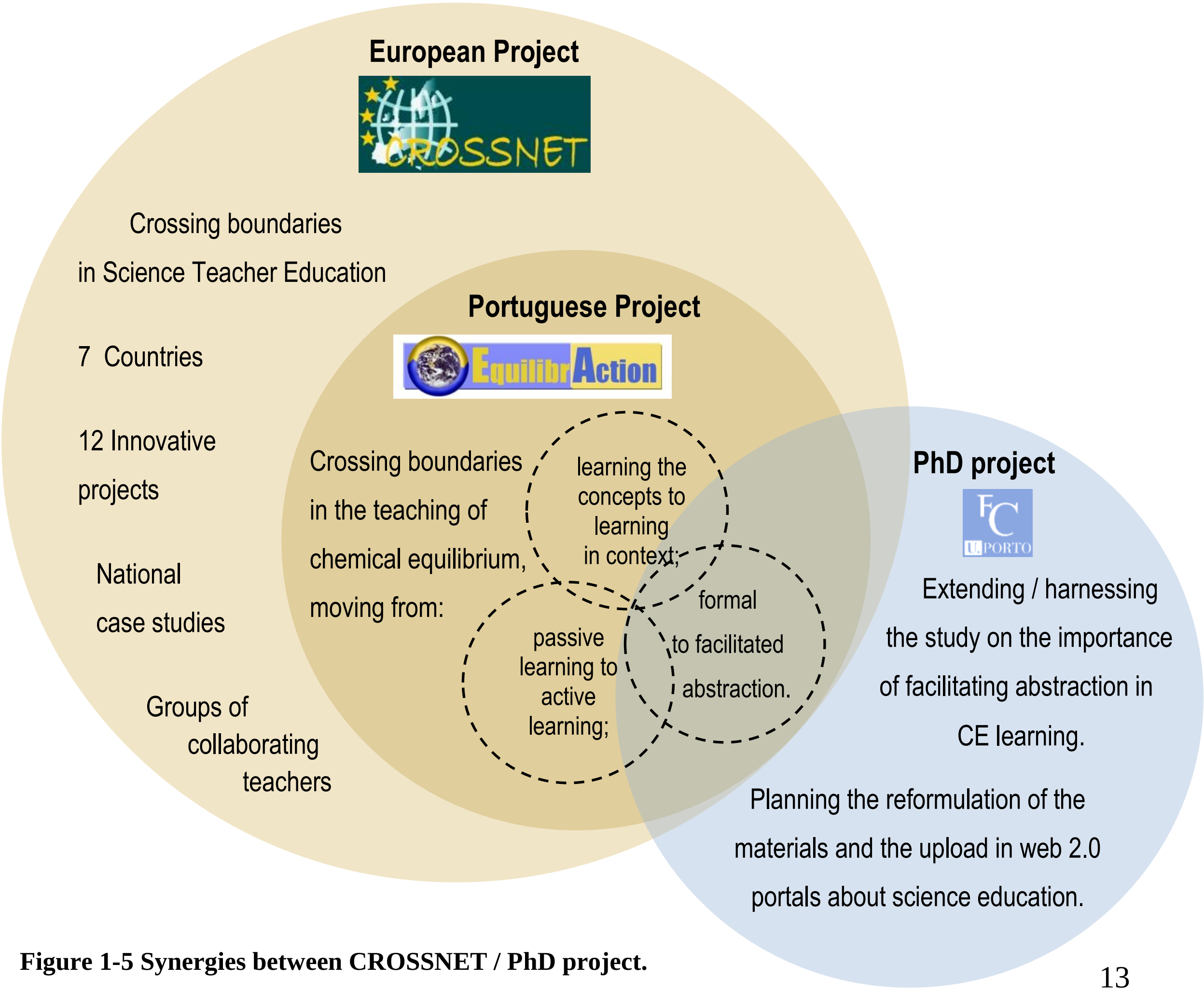


Figure 1-5 Synergies between CROSSNET / PhD project.

1.3. Main goals of the project

The broad purpose of this project is to develop an approach to take advantage from ICT's potential in the teaching of CE. Underlying to this general intention, the following goals/phases were initially associated to the project:

1. Considering the literature review on the specific nature of CE, learning difficulties in CE and "good practices" involving the use of ICT in the teaching of CE, we intend to outline the theoretical base for approaching the use of digital resources in the teaching of CE;

2. Developing synergies with CROSSNET project;

3. Design a pedagogical approach, centred in benefiting from the use of digital resources in the teaching of CE;

4. Collecting data over preponderant factors for taking advantage from ICT in the teaching of CE, by studying how the approach (designed in phase 3) works in the classroom context;

5. Gathering information for reformulating the approach and the resources included, in order to make the materials available online for the dissemination in the community chemistry teachers.

6. Based on the results of the study, suggest a list of recommendations to guide the use of digital resources in the teaching of CE.

As referred above, the intention of facilitating students' abstract reasoning, while approaching the use of digital resources in the teaching of CE, was an idea that became clear both from the literature review associated with the first specific objective presented and the collaboration in CROSSNET referred in the second. This fact led to the detailing and clarification of the central purpose of the project, which can be stated as:

Understand the circumstances that allow facilitating students' abstract reasoning in the learning of CE, through the design and implementation of a pedagogical approach incorporating the use of digital resources.

According to these purposes, several outcomes can be traced for this project:

- Innovation of pedagogical practices;
- Diversification of teaching resources;
- Recommendations on the use of digital resources in the teaching of CE;
- Guidance about how to support student's abstract thinking during the learning of CE;
- A "module" for teaching CE, available online.

In planning these goals, we have considered the current context in ICT, namely:

- the growing capability of new technologies for representation / interaction;
- the spread of Web 2.0 based platforms;
- the better technological equipping of the schools in recent years;
- the increase of time spent by young people in computer and online, imposing the internet as a mean for informal education.

1.4. Methodology overview

The FACE approach built under this project is supported by several studies in the area, as referred above and demonstrated by references presented in next chapters. Thus, it is expected that applying FACE approach in classroom context will lead to facilitated abstraction. Nevertheless, since this is a “prototype” approach, it is important to understand how it works in classroom context, analysing which features are relevant, difficulties in the process of transfer from theory to practice, aspects to reformulate…

The case study methodology is suitable when a researcher is looking for answers to questions such as "how" and "why?" In this work we proceeded to the construction of an innovative approach that had not been tested in context. Thus, it is relevant to investigate "how it works", getting to know the benefits and the weaknesses, as well as the factors that influence the process of facilitating abstraction.

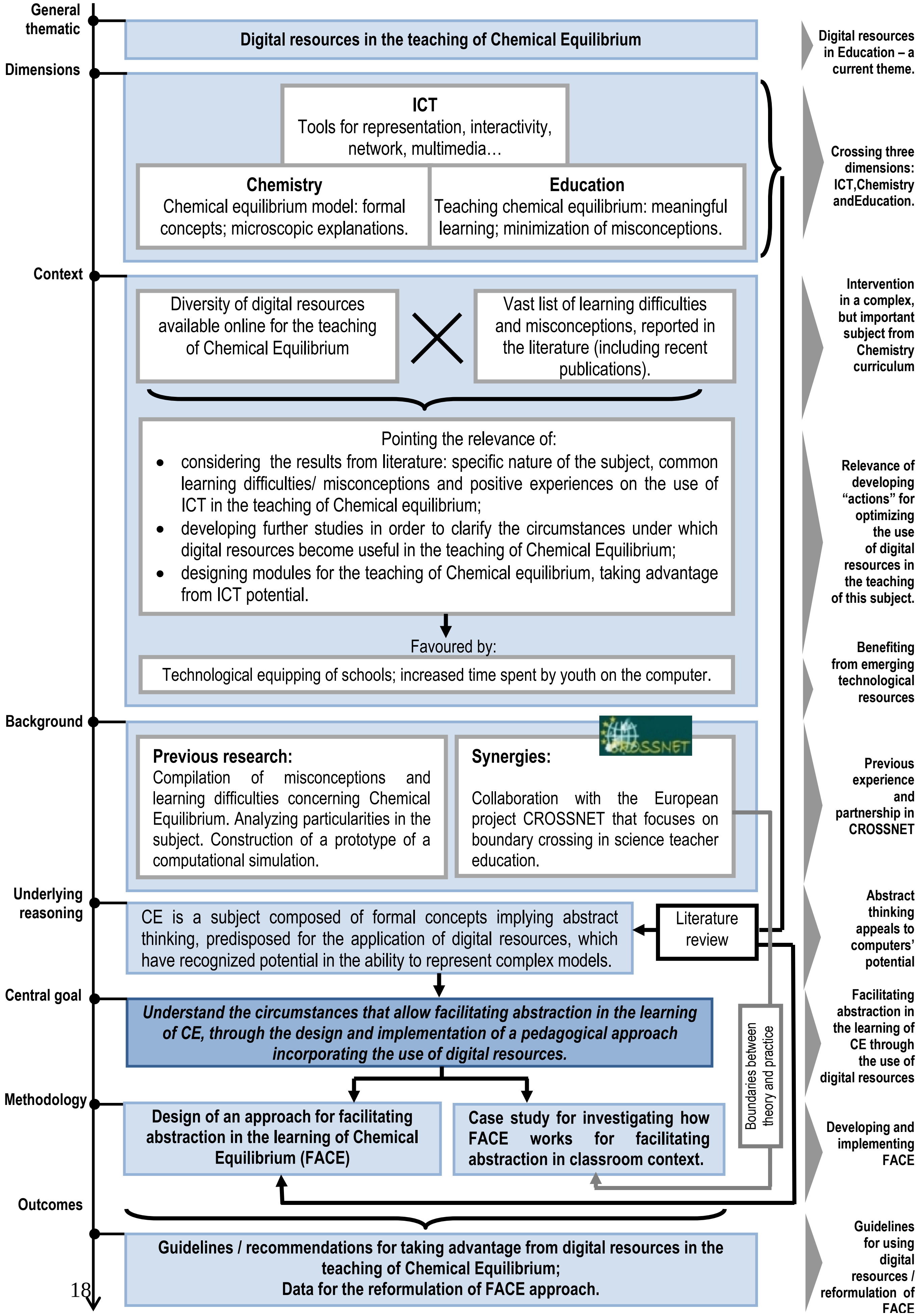
As seen in section 1.2, the overall theme of CROSSNET was the "border crossing in science education", which is compatible with the work on the boundaries between theory and practice and specifically the barrier of formal abstraction, associated with this PhD project. Thus, the importance to defining a common line of research between this PhD project and CROSSNET European project became evident.

Following this trail of thought, “case study” was selected as the methodology for investigation in this project:

- because the main focus resides in understanding the process of facilitating abstraction in CE learning, through the use of digital resources, answering to questions such as “how” and “why”;

- in order to benefit from the synergy whit CROSSNET project, where it was planned the conduction of cases studies in each of the participating countries.

At the end of this study it is intended to obtain guidelines / recommendations for the implementation of ICT in the teaching of Chemical Equilibrium, as well as data for the reformulation of the developed approach, a characteristic outcome from the case study methodology (Yin, 1994). In chapter 6 the investigative methodology will be presented in detail. Figure 1.6, summarizes the introduction to the project made along chapter 1.



General thematic

Digital resources in the teaching of Chemical Equilibrium

Digital resources in Education – a current theme.

Dimensions

ICT
Tools for representation, interactivity, network, multimedia…

Chemistry
Chemical equilibrium model: formal concepts; microscopic explanations.

Education
Teaching chemical equilibrium: meaningful learning; minimization of misconceptions.

Crossing three dimensions: ICT,Chemistry andEducation.

Context

Diversity of digital resources available online for the teaching of Chemical Equilibrium

Vast list of learning difficulties and misconceptions, reported in the literature (including recent publications).

Pointing the relevance of:

- considering the results from literature: specific nature of the subject, common learning difficulties/ misconceptions and positive experiences on the use of ICT in the teaching of Chemical equilibrium;
- developing further studies in order to clarify the circumstances under which digital resources become useful in the teaching of Chemical Equilibrium;
- designing modules for the teaching of Chemical equilibrium, taking advantage from ICT potential.

Favoured by:

Technological equipping of schools; increased time spent by youth on the computer.

Intervention in a complex, but important subject from Chemistry curriculum

Relevance of developing “actions” for optimizing the use of digital resources in the teaching of this subject.

Benefiting from emerging technological resources

Background

Previous research:
Compilation of misconceptions and learning difficulties concerning Chemical Equilibrium. Analyzing particularities in the subject. Construction of a prototype of a computational simulation.

Synergies:
Collaboration with the European project CROSSNET that focuses on boundary crossing in science teacher education.

Previous experience and partnership in CROSSNET

Underlying reasoning

CE is a subject composed of formal concepts implying abstract thinking, predisposed for the application of digital resources, which have recognized potential in the ability to represent complex models.

Literature review

Abstract thinking appeals to computers’ potential

Central goal

Understand the circumstances that allow facilitating abstraction in the learning of CE, through the design and implementation of a pedagogical approach incorporating the use of digital resources.

Facilitating abstraction in the learning of CE through the use of digital resources

Boundaries between theory and practice

Methodology

Design of an approach for facilitating abstraction in the learning of Chemical Equilibrium (FACE)

Case study for investigating how FACE works for facilitating abstraction in classroom context.

Developing and implementing FACE

Outcomes

Guidelines / recommendations for taking advantage from digital resources in the teaching of Chemical Equilibrium;
Data for the reformulation of FACE approach.

Guidelines for using digital resources / reformulation of FACE

Chapter 2 - Scientific Dimension: the concept of Chemical Equilibrium

2.1. About the nature of Chemical knowledge

> *"Still I had a lurking question.*
> *Would it not be better if one could really 'see'*
> *whether molecules as complicated as the sterols,*
> *or strychnine were just as experiment suggested?"*
>
> ***Dorothy Hodgkin, British biochemist (1910 - 1994)***

Our complex and rapidly changing world requires the ideas of chemistry for the understanding of its major aspects (Gilbert & Treagust, 2009). Chemistry, in a broad sense, is the study of matter and its transformations, a definition that can be traced back to its birth (Nature Chemistry, 2009).

In this chapter we will focus on discussing some aspects of the nature of chemistry, reason why we consider this review part of the scientific dimension of this thesis. Nevertheless, since our background is on chemistry education, as well as the main goal of this project, it is inevitable that we analyze chemistry's nature from an educational point of view, discussing the more relevant issues in the context of this study.

Chemistry obviously shares several features with other sciences, like the experimental component and the use of models to describe phenomena. Chemistry is usually referred as "the experimental science" (Tsaparlis, 2001). The practical nature of chemistry is mirrored in a closely connected industry (Sjöström, 2007). In fact, experimental details are important, but the theoretical rationale in which the experiment is conducted, is even more important (Tsaparlis, 2001). On the process of providing explanations for natural phenomena we impose our ideas of what might be important on the complexity of the natural world (Gilbert, 2005). Models are referred as a major part of the scientific enterprise (de Jong & Taber, 2014) and their development is crucial in the production of scientific knowledge (Gilbert, 2005). Modelling implies the transition from a first description of objects and events perceived by experience (phenomenology) to a second description using the world of theories and models (Tiberghien, 1994 cited in Dumon & Mzoughi-Khadhraoui, 2014). Models' importance is transversal to all science disciplines, but they are most important in chemistry because this subject involves many abstract and complex concepts (Halim et al., 2013), inexplicable without the use of analogies or models (Gabel, 1999). "Indeed, to a great extent, the theoretical content of chemistry is best seen as a set of models" (Taber, 2001). In chemistry "models refer to the theoretical entities, and the underlying assumptions, that are used to describe chemical systems by attributing to them some sort of internal structure, composition, and/or mechanism that serve the purpose of explaining or predicting the various properties of those systems" (Talanquer, 2011).

Chemistry is about knowing the properties of substances and how these relate to chemical structure and chemical bonding: these aspects are not separable (Barke & Wirbs, 2002). In chemistry the observed phenomena is reconceptualized not only at the macroscopic level but also in terms of the theoretical models of the structure of matter at the submicroscopic level (Dumon & Mzoughi-Khadhraoui, 2014). So, chemistry has a particular nature much related to its reliance on submicroscopic models, a notion that is well established in literature:

> "One of the essential characteristics of chemistry is the constant interplay between the macroscopic and microscopic levels of thought" (Sirhan, 2007).

> "For the chemist, models of the world at the submicroscopic scale of molecules, ions, and electrons do useful explanatory work, because the properties of those "particles" (i.e., the molecules, ions, electrons, etc.) are understood to interact to give rise to structures at the phenomenological macroscopic level, so they lead to the emergent properties that can be observed. This has long been a metaphysical premise of chemistry…" (de Jong & Taber, 2014).

> "…chemistry, to be more fully understood, has to move to the submicro situation where the behaviour of substances is interpreted in terms of the unseen and molecular and recorded in some representational language and notation." (Johnstone, 2000).
>
> "Teaching chemistry means discussing substances, their properties and reactions on the macroscopic level and structural models on the submicroscopic level." (Barke & Wirbs, 2002).
>
> "Chemistry deals then with a small (submicro) world, and at the same time a large world" (Tsaparlis, 2001).
>
> "One of the main ways in which these models are used in chemistry is to provide theoretical explanations at the molecular level which make sense of phenomena observed at the macroscopic level" (Taber, 2001).
>
> "The basis of the correct comprehension of chemical concepts is an understanding of the structure of matter" (Devetak et al., 2009).

In fact, for most of the topics, the chemist strives on the pursuit for microscopic explanation. There are other sciences, especially Physics, which also deal with submicroscopic considerations. In the literature the discussion about the relation/dependence between Chemistry and Physics is frequently present (Taber, 2001; Tsaparlis, 2001). It is usually recognized that chemistry is ultimately based around physical principles (Taber, 2001) and that physical methods became important to all chemistry fields (Tsaparlis, 2001). Nevertheless, different authors also safeguarded that chemistry plays a different role, related both to its creative purpose (transformation, production of new materials) and to the uniqueness of the level of explanation used. Several sentences from literature point out the creative nature of chemistry:

"Chemistry remains a very creative discipline - as Marcellin Berthelot once observed "chemistry creates its own object" (Nature chemistry, 2009).

"It is creative for example in the meaning that new molecules, with unique properties, can be created."(Christensson & Sjöström, 2014).

"Because of this capacity to synthesize new molecules and structures it is interesting to discuss whether chemistry is a science or a technology. (…) The existence of an own industry since a long time ago distinguishes chemistry from other sciences." (Sjöström, 2007).

About the uniqueness of the explanations, Taber (2001) notices the emergence of genuinely chemical concepts at the level of analysis that chemists are concerned with: "When new, higher level, concepts are developed from more fundamental principles, they are then able to provide a 'short-hand' that stands in place of the basic concepts." That is, chemistry's explanations are satisfactory for the claims of this science without having to reach the level of physics explanation. Both sciences can have the same principle but worth alone because they are helpful with their own models.

There is a creative nature in Chemistry and uniqueness in the level of explanation used: although ultimately based around physical principles, the emergence of genuinely chemical concepts stands out at the level of analysis that chemists are concerned with.

The "scale" appears to play an important role, although not exclusive in characterizing the level of explanation used in chemistry. Chemistry is usually positioned between physics and biology (Christensson & Sjöström, 2014). This classification is related to the application of chemistry in fields like technology and medicine, but is also associated to the level of analysis used to produce explanations in each of these sciences. "Positioned at the crossroads of the physical and biological sciences, chemistry deals with neither the infinitely small, nor the infinitely large, nor directly with life" (Hoffmann, 1995). This intermediary position of chemistry is considered in a simplistic notion of a hierarchy of sciences building upon each other (physics on maths, chemistry on physics, biology on chemistry, psychology on biology, etc.) (Taber, 2001). Jensen (1998) presents a hierarchical classification of sciences based on the scheme of Herbert Spencer (Figure 2.1). According to Jensen (1998) “Sciences higher in the hierarchy make use of principles established by those lower in the hierarchy, though at each level new forms of organization appear. The concrete sciences deal with specific classes of objects or bodies found in the universe, whereas the abstract sciences attempt to establish universal principles applicable to all of these bodies.”

The importance of “scale” in chemistry, becomes clear, for instance, in the debate that took place around the Nobel Prize in Chemistry for 2009, which was awarded for research into the structure and function of the ribosome: “The ribosome, however, falls in the grey and ‘fuzzy’ area in the middle: too large for every chemist to see its relevance, but too small to be classified purely as biology” (Nature Chemistry, 2009). Notwithstanding the fact that chemistry includes macro models and an increasingly important knowledge at quantum level in modern chemistry, we can assume that “The core of chemical theory is the dynamics and structure of matter on a molecular level.” (Sjöström, 2007).

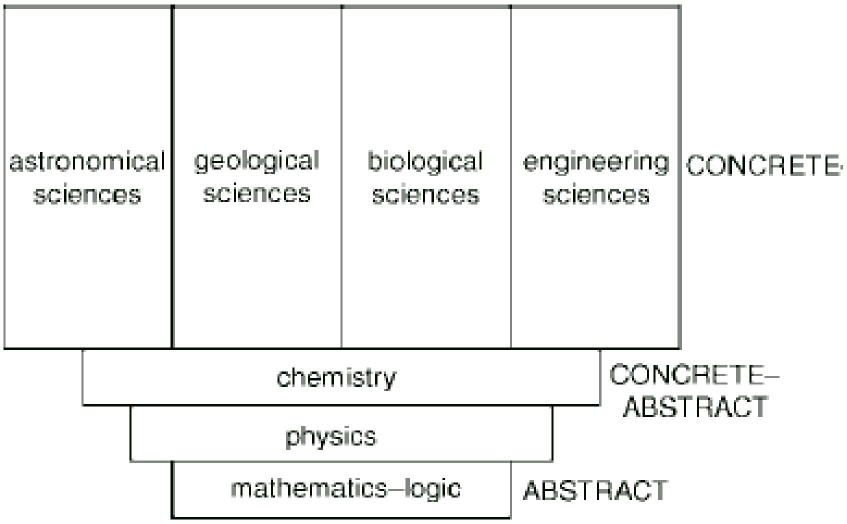


Figure 2-1 A hierarchical classification of sciences based on the scheme of Herbert Spencer (after Jensen, 1998).

The fact that the ultimate explanations for chemical phenomena rely on physical principals, remember us that models in modern Physics can go into a level of analysis positioned even in a smaller scale than great part of the explanations used in chemistry. Nevertheless, at a secondary school level, most of the Physics lays around the description of macro scale events supported on mathematics. It is possible to study great part of physics with a brick (Johnstone, 1982). Newtonian models are still largely applied in Physics teaching (Taber, 2001). In opposition, at the school level of chemistry, asking “why” leads frequently to submicro explanation, an event that doesn’t happen in Physics with the same frequency. So, the relevance that the submicro level has in the teaching of chemistry is unrivalled. In most of chemistry’s subjects, the submicroscopic level assumes the status of essential condition for a satisfactory explanation.

The relevance of the submicro level in Chemistry is unrivaled by other sciences, especially at secondary school level. For most of Chemistry’s subjects, the submicroscopic level of explanation is determinant in the model used to describe the phenomena and an essential condition for a satisfactory explanation.

Another characteristic of chemistry is the use of a specific language based on rules and/or conventions (Dumon & Mzoughi-Khadhraoui, 2014). This mathematical/symbolic “world”, used to express relationships at the macroscopic and microscopic levels, constitutes an additional factor to the complexity of chemistry (Gabel, 1999).

Chemistry has a specific language used to express relationships at the macroscopic and microscopic levels, an additional factor to the complexity.

Johnstone (1982) referred that academic chemists view their subject at least at three different levels, which he initially names: descriptive and functional, representational and explanatory. Later, Johnstone presents these levels as the corners of a triangle (Figure 2.2) and associates the above mentioned designations with macro, symbolic and submicro “worlds” (Johnstone, 1991; 2000). Talanquer (2011) reports to these levels as:

- *Descriptive and functional* level, related to “macrochemistry”, at which phenomena are experienced, observed, and described.

- *Representational* level in which symbolic language is used to represent and communicate concepts and ideas.

- *Explanatory* level, related to “submicrochemistry”, at which phenomena are explained.

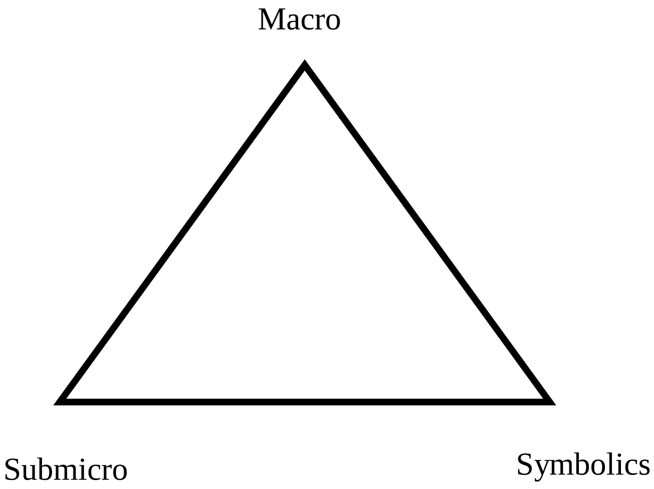


Figure 2-2 The triangle of Chemistry (after Johnstone, 1991).

Johnstone (2000) refers to this view about chemistry in the following words: “I believe that it exists in three forms which can be thought of as corners of a triangle. No one form is superior to another, but each one complements the other. These forms of the subject are (a) the *macro* and tangible: what can be seen, touched and smelt; (b) the *submicro*: atoms, molecules, ions and structures; and (c) the *representational*: symbols, formulae, equations, molarity, mathematical manipulation and graphs.

This idea has become a reference for discussing several issues in chemistry education (Dumon & Mzoughi-Khadhraoui, 2014; Sirhan, 2007; Talanquer, 2011) and has been adopted by many chemistry educators, curriculum designers, and researchers (de Jong & Taber, 2014) This framework has been recently designated “triplet relationship” (Gilbert & Treagust, 2009). Several statements from literature show the acceptance of this triplet nature of chemistry:

> "During the learning of chemistry, the constant interplay between these three levels of thought…" (Dumon & Mzoughi-Khadhraoui, 2014).

> "This relationship plays a more dominant role in chemistry than in the other natural sciences" (de Jong & Taber, 2014).

> "…helped us to see that the three learning levels, (the symbolic, macroscopic and submicroscopic, or molecular) are needed for students to make sense of chemistry"(Mahafy, 2004).

It has served as a framework for many research studies in chemical education and as a central idea in various curriculum projects, constituting guidance for teachers and software developers (Talanquer, 2011). Different publications refer to the idea, reflect about it or propose adaptations through the years (Christensson & Sjöström, 2014; de Jong & Taber, 2014; Gabel, 1993, 1999; Halim et al., 2013; Mahafy, 2004; Meijer, 2011; Ozmen, 2011; Taber, 2013; Talanquer, 2011; Tsaparlis, 2001), including several recent publications, which seem to show that a renewed attention is being driven to the triplet relationship. The initial idea is still "generally accepted" (Dumon & Mzoughi-Khadhraoui, 2014) and frequently used as a starting approach (de Jong & Taber, 2014). The three corners of the triangle are labelled in different ways in literature such as levels of representation, types of knowledge; worlds, levels of description or thought... (Talanquer, 2011). We will apply, from now on, the designation "levels", first used by Johnstone, back in 1982.

As Talanquer (2011) states “this triplet view of our chemical knowledge has been adopted and adapted by many people who, through personal or collective reinterpretations, have generated what can be identified as different faces, personalities or manifestations of the triplet.”

Chemistry’s particular nature is well accepted to be related to the triplet relationship: coexistence of macroscopic, submicroscopic and symbolic levels of knowledge – a triangle that plays a more dominant role than in any other science.

Although the utility of this framework in highlighting the main components of chemical knowledge, some caution is recommended in its application and interpretation (Talanquer, 2011). Talanquer critically reflects on the different adaptations, safeguarding that “different views tend to challenge and enrich our understanding of the nature of chemical knowledge”.

One of the critics made to the triangle of Johnstone is the lack of a clear place for models that are based in macro considerations: “by only focusing on the particulate models of matter (*submicro*) in the explanatory component, Johnstone’s triplet seems to exclude the wide variety of macroscopic theories and models that chemists use to explain and predict the properties of substances and chemical processes (e.g. chemical kinetics and thermodynamics)” (Talanquer, 2011). Talanquer (2011), reports that in some studies the macro level seems to include both the actual phenomena and the concepts used to describe them, while other authors separate the empirical (macro) level of the experienced phenomena from the modelling (macro) level. In fact, if this level is considered conceptual, can it be labelled as purely descriptive, or as partly explanatory? From a pedagogical perspective, central to this project, it is import to acknowledge the various meanings attributed to the macro level in the chemical education literature (Talanquer, 2011).

Taber (2013) separates the experiential level of the phenomena from the models used to interpret it, calling this process/product as “macroscopic conceptualization” (Figure 2.3).

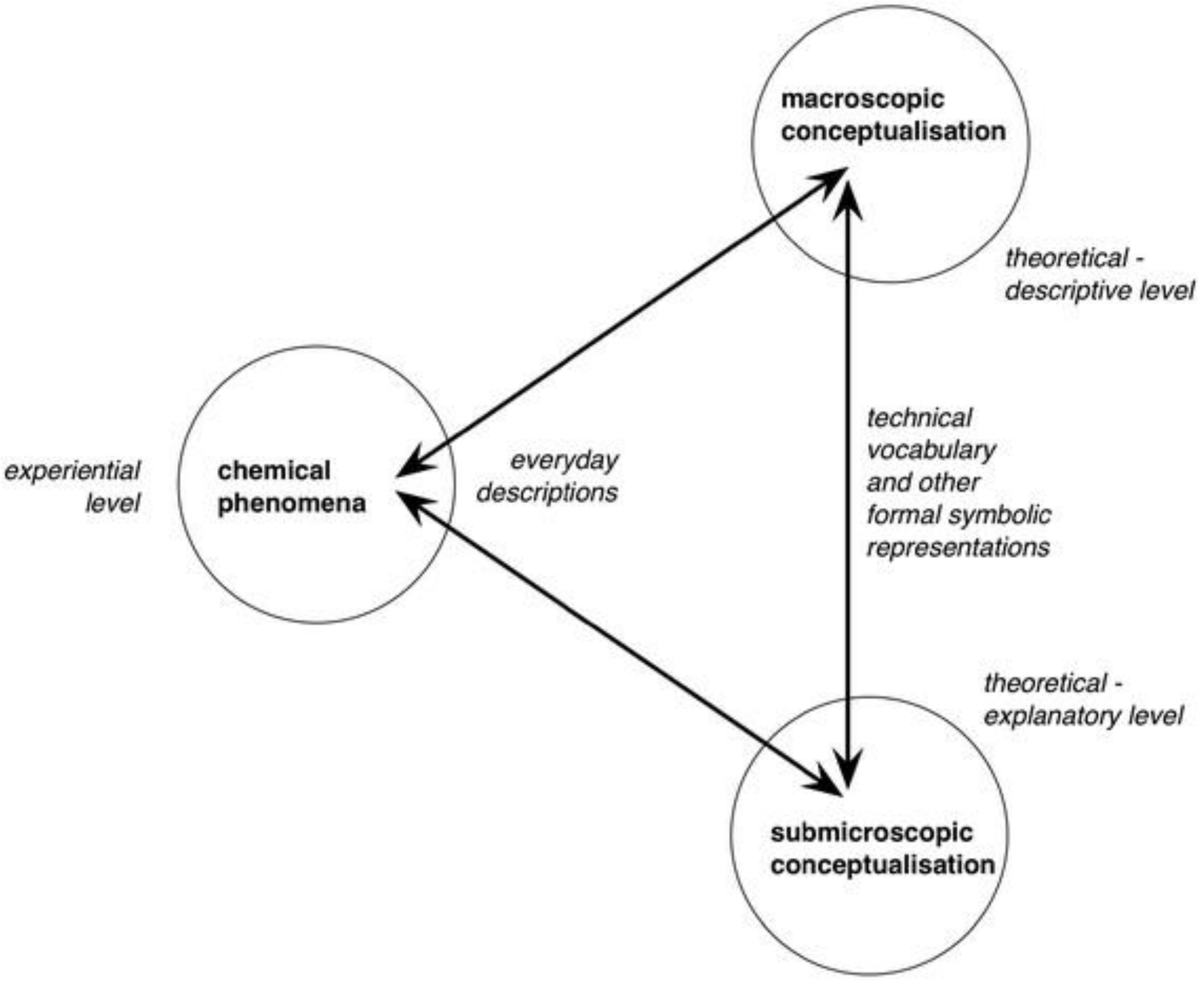


Figure 2-3 "Re-descriptions" (represented by the arrows) between direct experience and formal representations of the conceptualization of the subject at two distinct levels (after Taber, 2013).

In this framework, the observed phenomena is reconceptualized both at the macroscopic level and in terms of the theoretical models of the structure of matter at the submicroscopic level. This idea is accepted by other authors (Dumon & Mzoughi-Khadhraoui, 2014). Following this trail of ideas, we come to the conclusion that learning chemistry involves re-descriptions (represented by the arrows) between the everyday language of direct experience and formal representations of the conceptualisation of the subject at two distinct levels (Taber, 2013).

The symbolic level of Johnstone (1991) loses the character of independent level in Taber's (2013) approach, becoming a bridge between macro and submicro levels (Figure 3). According to Taber (2013), the symbolic knowledge domain cannot be readily separated from the macroscopic and submicroscopic domains, it is inherent in how we think about chemistry. In fact, an important characteristic of the "symbolic world" that we use in chemistry, is that a major part of the symbolic representations refer to both concepts at the macro level (substances) and to the submicro (atoms, molecules, etc.) according to the interpretation made (de Jong & Taber, 2014).

The symbolic corner in Johnstone's triplet has also been a target of other discussions and adaptations through the years. The semi-symbolic, semi-iconic nature of many visual representations is one of the "ambiguities" reported (Talanquer, 2011). Visual representations in chemistry seem to stay between symbols and models: between a way to communicate concepts and ideas and actual attempts to represent things. This hybrid status is an uneasy one (Hoffmann & Laszlo, 1991; Talanquer, 2011). Several sentences from literature show this unclear nature of the symbolic level in chemistry, between formal communication and "support" for conceptualization:

> "In order to represent the concepts … chemists use conventional formalisms: chemical symbols and formulae, particulate drawings, molecular models, drawings of chemical apparatus, etc. (Dumon & Mzoughi-Khadhraoui, 2014).
>
> "Representative chemistry is useful in making sense of learning to use chemical concepts." (de Jong & Taber, 2014).
>
> "As the discipline has developed, chemists have created different representations to develop a comprehensive understanding of chemical concepts, for example, molecular structure and reactivity". (Stull et al., 2012).
>
> "Symbolic levels of chemical concepts [symbols of elements, chemical formulae and equations, mathematical equations, graphical representations such as submicro representations of particulate level of matter (SMR), different models, schemata, etc.] are used by scientifically literate people to easily communicate about the phenomena at abstract level"(Devetak et al., 2009).

The concept of representation was described (many years ago) by Peirce (1955, cited in Potgieter et al., 2008), stating that for a notation to function as a representation, someone has to interpret it and give it meaning. So, there are some doubts about placing chemistry's representations in the symbolic level, considering them just as signs for communication, or in the submicro level when we see some explanatory power on them (Talanquer, 2011). Dumon and Mzoughi-Khadhraoui (2014) base their adaptation to the triplet relationship on Taber's model but they "solve" the ambiguity of symbolic level by proposing the separated "existence" of a level with the broader designation of "visualization". Dumon and Mzoughi-Khadhraoui (2014) proposed a tetrahedron that the authors called the "expanded chemistry triplet" (Figure 2.4).

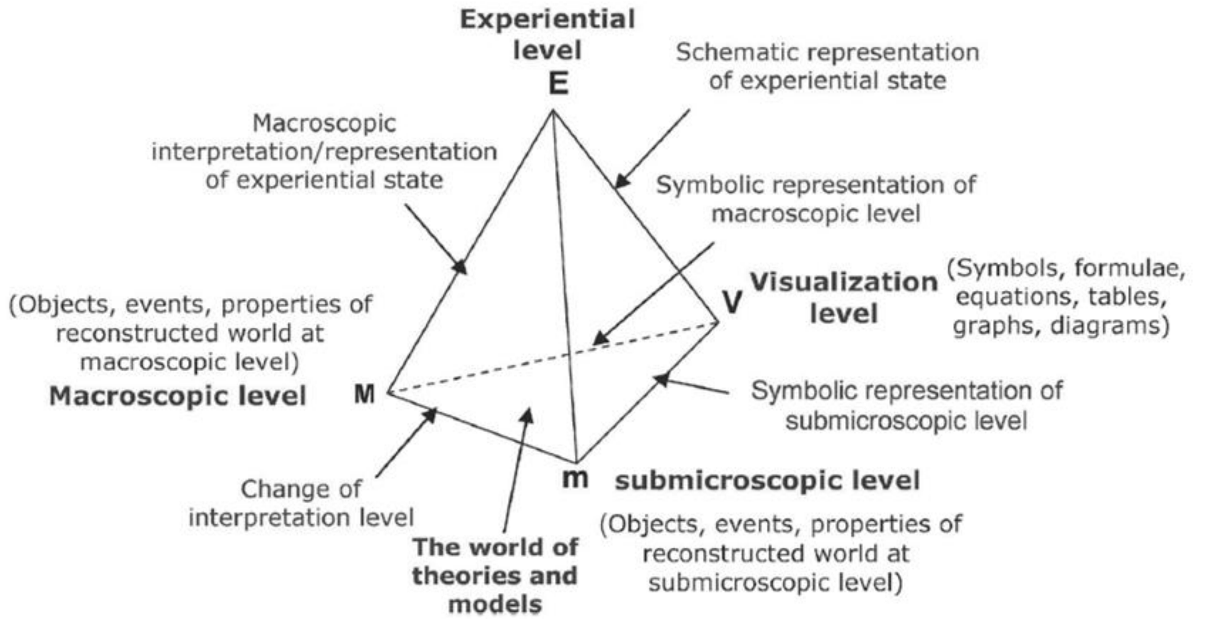


Figure 2-4 Expanded chemistry triplet (after Dumon & Mzoughi-Khadhraoui, 2014)

In this adaptation there is present an experiential level like in Taber's approach. Nevertheless there is also included the "visualization" level. Common language is used in the first description of experiential state (apex E) that involves only perceptual phenomena. In the base of the tetrahedron there are the theories and models. These authors also link each of the vertexes explaining the meaning going along edges in the MEV and MVm triangles:

- EM - corresponds to the first step in modelling that is to enable students to describe the experiential facts using the language of chemistry, neglecting a number of perceptual phenomena to focus on the change in the kinds of chemicals.

- VM - the next step is the representation of the macroscopic level trough qualitative symbolic language (first level of representation) and then trough symbols that allow to understanding composition (a second level of representation).

- EV – corresponds to the representation of the experiment by a drawing.

- Vm – refers to the moving to the submicro level in order to understand the representations used.

- Mm – corresponds to a change in the modelling level.

Dumon and Mzoughi-Khadhraoui, 2014 also state that the quantitative interpretation of the observed changes requires the experiential data (masses, volumes: apex E) to be linked with the world of theories and models (connection between the triangles MEV and MVm).

Now we move to some reflection about the "submicro" corner of the triplet relationship. Ben-Zvi, Eylon, and Silberstein (1988, cited in Talanquer, 2011) considered three distinct levels of description of matter: the *macroscopic* (of the phenomena), the *atomic molecular* (one single-particle), and the *multi-atomic* (many particles).So, some doubts have been raised about the scale of the submicroscopic level: is it referent to single particles or/and also to the interactions in multi-particle models?

Jensen (1998) also distinguished several scales, instead of restricting chemical knowledge to macro and micro levels: molar, molecular and electronic levels; and three dimensions: composition and structure, energy, and time. Molecular level is considered "powerful", nevertheless it leaves many questions unanswered, namely explanation for the observation of variations in properties that cannot be traced to a change in either the kind, number, or arrangement of the atoms (Jensen 1998). Jensen (1998) summarizes in a table the type of knowledge resulting from crossing each scale with each dimension. In table 2.1 we present a "pocket" version of the table presented by Jensen (1998).

Studies of this kind reveal the "multi-layered nature of the explanatory level in chemistry" (Talanquer, 2011).

Table 2-1 The logical structure of chemistry, adapted from Jensen (1998).

		Dimensions		
		Composition and structure	Energy	Time
Levels	Molar	Composition of substances, solutions and mixtures.	Calorimetric entropies and heats of formation. Free energies and equilibrium constants.	Experimental rate laws and entropies and heats of activation.
	Molecular	Absolute and structural formulas.	Molecular interpretation of entropy, average bond energies, etc. Molecular mechanics.	Molecular reaction mechanisms. Molecular view of activation entropies and activated complexes.
	Electrical	Lewis structures. Variations in either electronic or nuclear composition	Calculation of energies based on electronic structure. Interpretation of spectra.	Isotope effects. Calculation of activation energies. Electronic reactivity indices.

Meijer (2011) focuses on the perspective of the chemistry's learner, concluding that the mental task of jumping between the macro domain and the submicro domain is very hard for many students. In his works, a "meso level" is proposed to bridge between macro and submicro levels (Meijer, 2011). According to the author "Structures of materials at meso level can be used to facilitate the students' understanding that properties of a system come into view as a result of underlying interactions among components of that system".

This idea can be considered as an extension of the usual triangle of meanings into a tetrahedron of meanings (de Jong & Taber, 2014) (Figure 2.5).

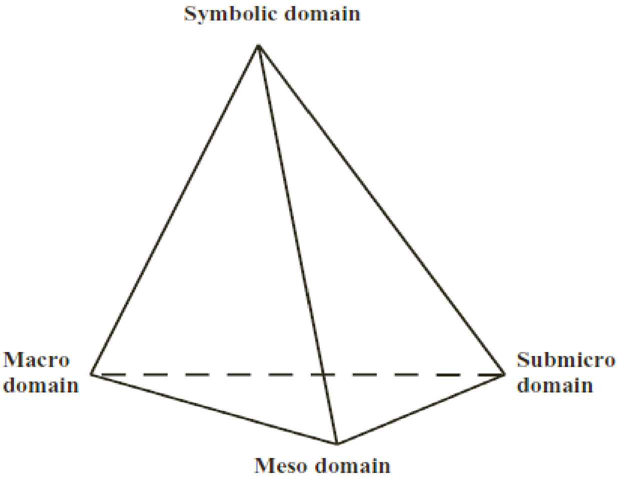


Figure 2-5 Tet¬rahedron of meanings that results from Meijer's (2011) addition a meso level to bridge the gap between macro and micro levels (after de Jong & Taber, 2014).

Another limitation pointed in the triplet relationship is the missing role played by the context and the individuals involved in the process. It has been suggested that a fourth component, the human element, should be added to integrate the learning of the discipline within contexts in which chemistry affects the lives of citizens and communities (Talanquer, 2011).

Mahaffy (2004) refers that the original triangle "has been used effectively in the last decade to describe what we value in teaching and learning about the world of atoms and molecules". Mahaffy (2004) suggested the placement of the human component in the triplet relationship in order to address concerns about scientific literacy and limited public understanding of the role of chemistry in everyday life: "The fourth vertex represents the web of human contexts for learning chemistry – the human element" (Mahaffy, 2004) (Figure 2.6). The fourth vertex places new emphasis on two dimensions of learning chemistry: teaching in context (technology, environment...) and the concerns with the human learner (difficulties, pedagogical strategies...) Mahaffy (2004). We will develop this idea in Chapter 3.

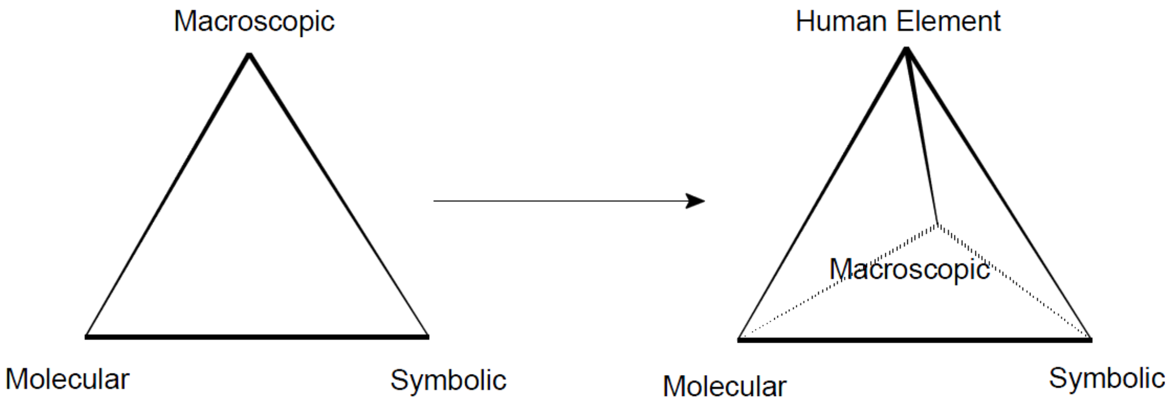


Figure 2-6 Tetrahedral chemistry education: A new emphasis on the human element (after Mahaffy, 2004).

Talanquer (2011) questions if the human component should be considered as a fourth level to be added to the triplet or seen as a particular approach to the way in which the other three levels can be introduced, explored, and discussed in the classroom: “if we need to add a human component to the triplet relationship, why not also consider philosophical, historical, or technological components?”. Sjöström (2013, cited in Christensson & Sjöström, 2014) subdivided the tetrahedron into three levels: applied chemistry (Level 1); socio-cultural context (Level 2); and a critical philosophical approach (Level 3) (Figure 2.7).

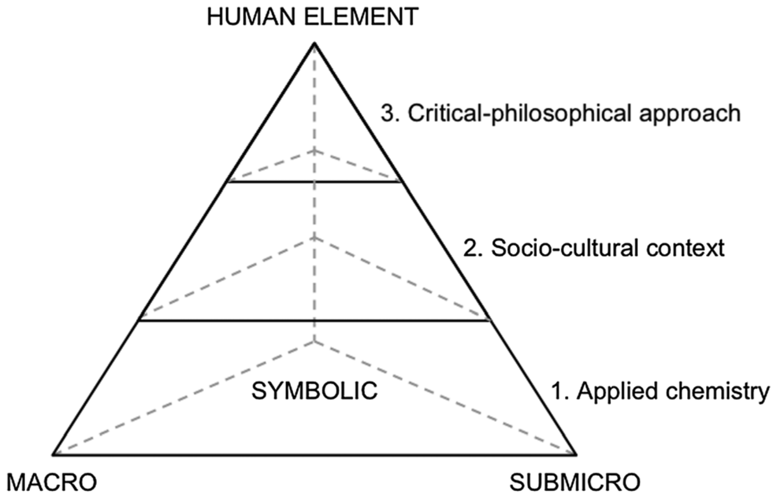


Figure 2-7 Tetrahedron of meanings subdivide by Sjöström (2013, cited in Christensson and Sjöström, 2014).

Talanquer (2011) also presents his model stating “I will not resist the temptation to generate my own pedagogical interpretation of the nature and structure of chemical knowledge.” He suggests that the chemistry knowledge that is relevant for teaching can be characterized as being of three main “types”:

- *Experiences* - related to the descriptive knowledge of chemical substances and processes, a type of knowledge mainly of empirical character.

- *Models* - includes descriptive, explanatory, and predictive theoretical models that chemists have developed to make sense of the experienced world.

- *Visualisations* - encompasses the static and dynamic visual signs (from symbols to icons) developed to facilitate qualitative and quantitative thinking and communication about both experiences and models in chemistry.

Talanquer (2011) also distinguishes between the experience and the model, considering them two types of knowledge between whom students need support for translation. For the third type of knowledge, Talanquer (2011) chooses the designation “visualizations”, like Dumon & Mzoughi-Khadhraoui (2014), and describes them as a type of knowledge that includes: “chemical symbols and formulas, particulate drawings, mathematical equations, graphs, animations, simulations, physical models, etc., used to visually represent core components of the theoretical model".

But Talanquer (2011) proposes a model that goes further than enunciating and relating and the main types of chemical knowledge: "Given that chemists explore, model, and build visualizations of the properties and behaviour of matter at different length scales, from the macroscopic to the subatomic, one can argue that each of the three main types of knowledge just described span these multiple scales or levels" (Talanquer, 2011). So, the tree types of knowledge can be conceptualized in multiple scales (Figure 2.8).

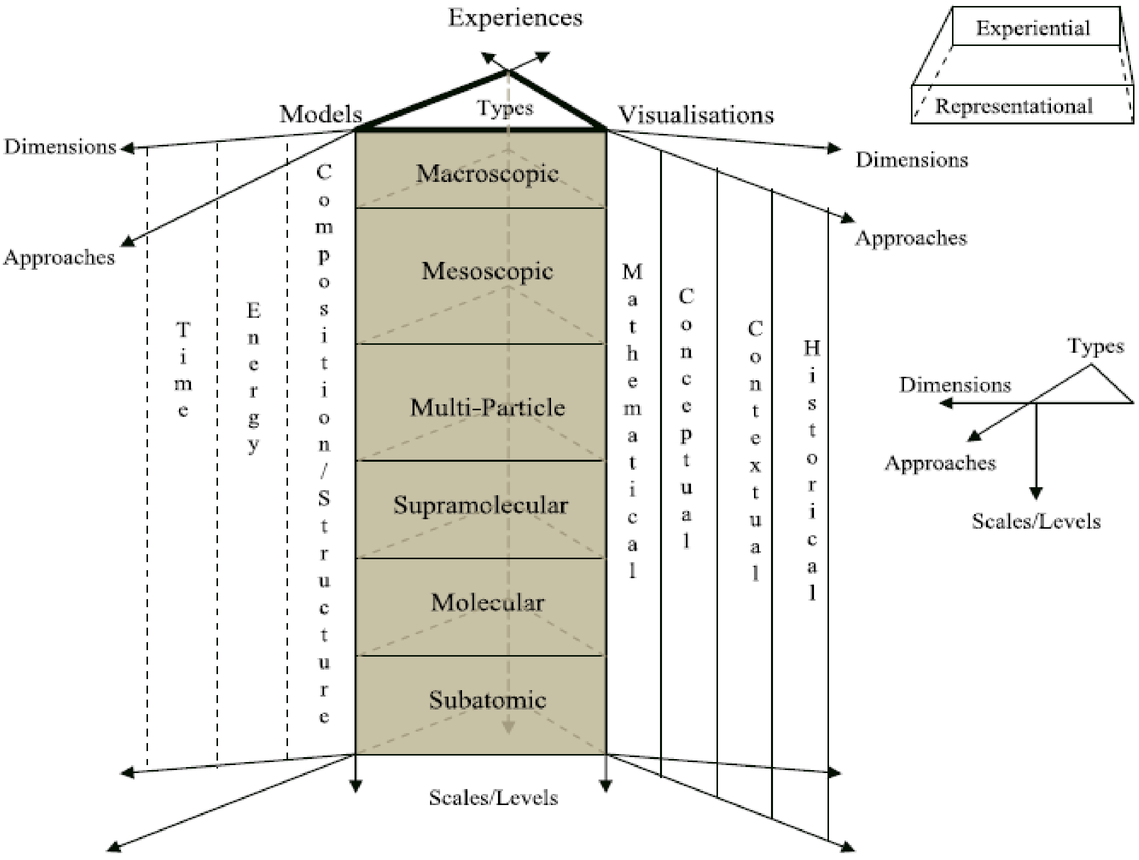


Figure 2-8 Chemistry knowledge space (after Talanquer, 2011).

Talanquer (2011) also recovers the dimensions from Jensen (1998) grid, including them in this framework, as well as several approaches that can be used to "reach" chemistry. According to Talanquer, figure 2.7 "reinforces the idea that beyond the ability to translate between different visualization forms, meaningful chemistry learning requires students to be able to translate within and across knowledge types, scales, dimensions, and approaches.”

Talanquer (2011) justifies the multiple entrances of his framework with the confusion that arises from merging categories: “Without neglecting the interrelationships among the types, levels, dimensions, and approaches … more problems and confusions seem to arise from trying to merge categories or build rigid links between them (e.g. symbolic with mathematical; submicroscopic with conceptual; experiences with macroscopic) than from granting them some degree of independence”.

In the present study, the base model from Johnstone will be used in the next chapters to discuss the knowledge and reasoning involved in the learning of CE, as well as the nature of the misconceptions in the field. Nevertheless, maintaining the same triangular structure of the initial triplet relationship, we would like to expand the idea, fruit of this literature review and our own interpretation and experience (Figure 2.9). Talanquer (2011) defends that this is the “type of personal reconstruction of knowledge and understanding that science educators should be encouraged to do to enhance and develop pedagogical content knowledge in a given discipline.”

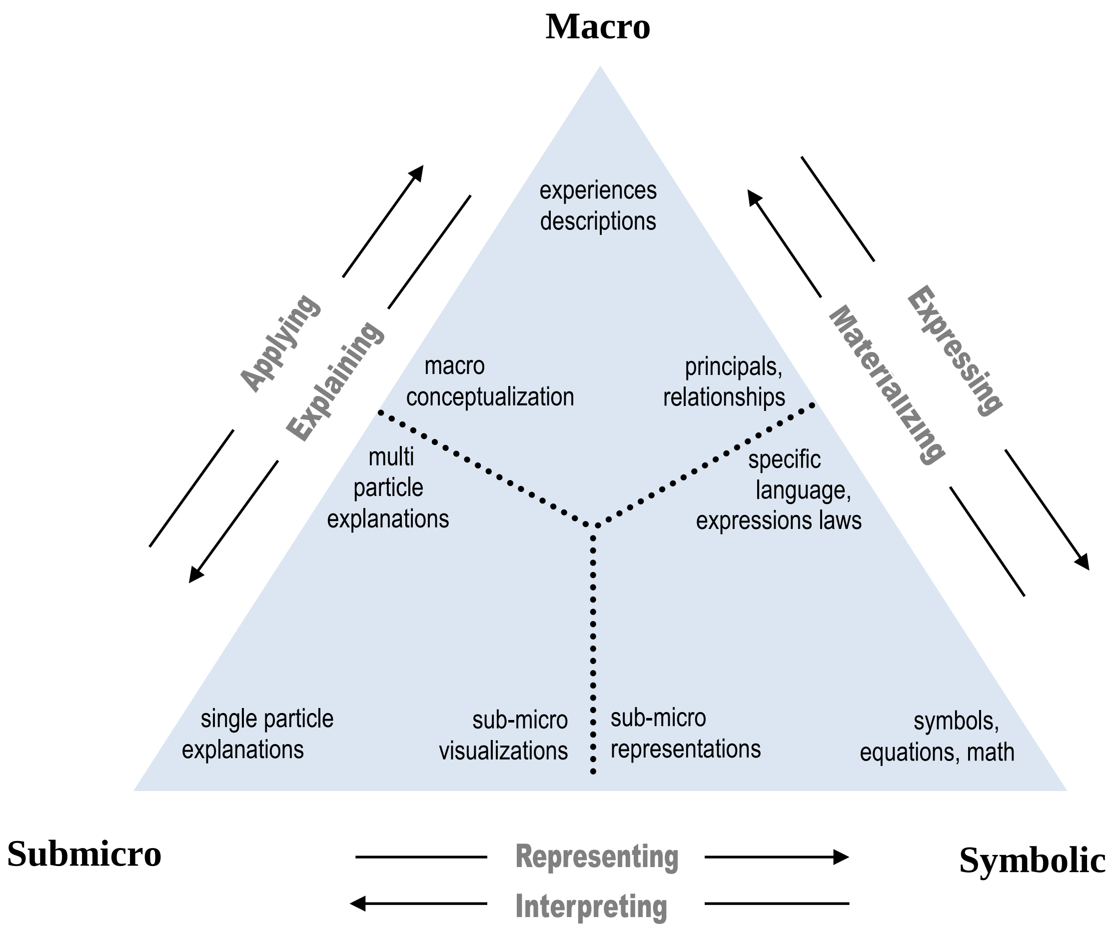


Figure 2-9 Zones of Chemistry knowledge space – an expansion to the scheme proposed by Johnstone (1991).

The first feature of our expansion is attributing meaning to the inner triangular area in Johnstone's (1991) relationship. Each point inside this area represents a particular combination of macro, micro and symbolic character. With this approach we can "locate" processes used in chemistry, knowledge produced and even concepts, in accordance with their particular relation to the different levels. In this framework, it is possible to divide the triangle in three equal areas, marking the zones where each level is dominant (bounded by dotted lines in Figure 2.9). Only the knowledge/processes located in the vertices of the triangle can be considered having an entirely macro, submicro or symbolic character. As we step away from the vertices, the mixed character grows, incorporating features from the different levels. We intend to use this representation, as a metaphor to show that the content of chemistry frequently has a mixed nature: some processes and knowledge mainly connected to one of the levels can be close to the domain of another level.

Several authors notice the dependence and intersection between the levels in Johnstone (1991) approach:

> “It is eventually very hard to separate this levels” (Johnstone, 1982).

> “the symbolic knowledge domain cannot be readily separated from the macroscopic and submicroscopic domains…” (Taber, 2013).

> “Chemical formulae should be considered as shortened models of the structure of substances on the submicro level, structural models could even be regarded as mediators between phenomena and chemical symbols.” (de Jong & Taber, 2014).

> “the interactions and distinctions between them (the levels) are important characteristics of chemistry learning and necessary for achievement in comprehending chemical concepts” (Sirhran, 2007).

Sentences like the ones above support our expansion from simple vertices of absolute macro, micro or symbolic nature to zones of dominant macro, micro or symbolic character (Figure 2.10). The vertices in our approach represent now possible particular cases.

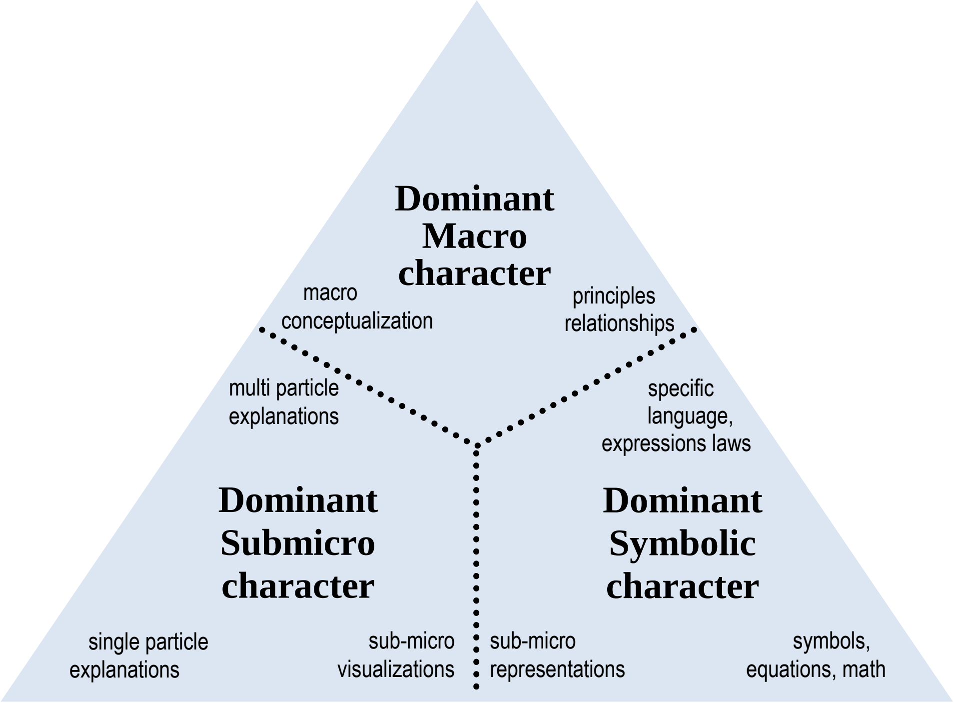


Figure 2-10 Zones of dominant macro, micro or symbolic character in Chemistry knowledge space.

With this expansion we intend to solve some of the limitations pointed to Johnstone triangle, preserving most of the original framework:

1. In the literature it's referred the missing place for macro models in the triangle of chemistry presented by Johnstone (1991), since the macro level is considered descriptive in the original triangle. Some authors propose the separation in an experiential level related to the description of the phenomena and a macro level related to conceptualization in macro/molar scale (Taber, 2013; Dumon & Mzoughi-Khadhraoui, 2014). Also, some publications consider this level to have both experiential and explanatory character (Talanquer, 2011). In our expansion, the idea of a macro dominant area leaves room for conceptual processes at this level that we label "macro conceptualization". Since we consider this kind of processes to be closer to the knowledge typical from the micro level due to its conceptual character, we place it in the macro dominant area but close to the micro area, attributing to it some mixed character. The more empirical experiences also have a place inside the macro level, but closer

to the vertex that represents the pure macro character. Still placed in the macro dominant zone but close to the symbolic level are the relationships and principles which express knowledge acquired at macro level.

2. The uncertainty in the scope of submicro scale is an observation usually made to Johnstone's approach, since models in chemistry span through different scales. Some authors include "electrical" to multi particle levels of knowledge (Jensen, 1998; Meijer, 2011; Talanquer, 2011). Another feature of the framework from Figure 2.9 is allowing the micro level to include models from several scales. Larger scale explanations stay close to the macro dominant zone, while models increasingly based in more fundamental principles tend to the submicro vertex. In the context of this expansion, the meso level proposed by Meijer (2011) could be placed in the dividing line between macro and submicro levels.

3. Another observation made to the triplet relationship is the ambiguity of symbolic level as including representations that support models or just codes for communication. Some authors prefer to use the word "visualizations" when referring the representations used in chemistry (Dumon & Mzoughi-Khadhraoui, 2014; Talanquer, 2011). Others consider representations as a bridge between macro and submicro levels (Taber, 2013): "The symbolic is inherent in how we think about chemistry". We argue that submicro representations aren't restricted to an entirely symbolic nature but have a dominant symbolic character. So, we include them in the symbolic dominant zone but close to the submicro domain. We also use the word visualizations. Nevertheless, we consider visualizations to have a closer relation to the submicro explanations used in chemistry, thus placing them in the submicro domain right next to the symbolic zone. Near to the symbolic vertex we place the instruments used in chemistry. So, the symbolic dominant knowledge can include both representations that are close to the visualization chemists make

> about the submicro "world" and the more purely symbolic instruments like symbols, equations and mathematics. Finally, in the symbolic area next to the macro level, we place the specific language and the mathematical laws used to communicate and quantify in chemistry.

Another feature that we add to this model, results from the reflection upon the major purposes of moving between the levels. Based on our own experience and supported by some "thoughts" from literature we select the main (not exclusive) "action" involved in each move between the levels. So, the arrows around the triangle in Figure 2.9 express the usual activity performed by the subject (the student, from the viewpoint of chemistry education) when moving from one level to another.

We label the action performed when "traveling" from macro to submicro level as "explaining". So, when moving from macro descriptions to the submicro models there is usually the intention of explaining phenomena. Several publications, including initial references from Johnstone (1982; 1991) refer the explanatory character of submicro level in chemistry being in accordance to our choice. Johnstone (1982) addresses micro level, as the level necessary to explain why chemical substances behave the way they do. De Jong and Taber (2014) argue that chemistry teaching frequently starts from an observable phenomenon and then explains it in terms of atomic structure and intermolecular interactions. In the opposite direction, while moving from the submicro level to the macro level, the theoretical knowledge is applied to predict events on the empirical world, plan experiments, produce new materials…

It has already been referred that the symbolic level is seen as a bridge between macro and submicro levels: "A key subset of the symbolic representations used in chemistry allows us to bridge *between* the macroscopic phenomena and the theoretical models posited at the submicroscopic scale" (de Jong & Taber, 2014). The words represent and communicate are frequently used when speaking about this level's role:

- "We need to use symbolic language to communicate chemistry taught at the macroscopic level" (de Jong & Taber, 2014);

- symbolic domain is concerned with representing and communicating the concepts and models developed at the other two levels (Taber, 2013).

For the arrow along the submicro to symbolic edge we chose the designation "representing", since most of the submicro models make use of representations of symbolic character as a framework. The mathematical instruments are also a part of the symbolic level, which includes mathematical equations, ratios, expressions, quantitative relations… Thus, we have decided to name "expressing" the arrow approaching symbolic level from a macro perspective in order to include both the meanings of communicating through a specific language and formulating the relations between substances and their properties through the use of mathematics.

For the paths that go from symbolic level to the remaining levels, we start by noticing that symbolic language acquires different meanings whether analyzed form submicro or macro viewpoints (de Jong & Taber, 2014). So, we consider "interpreting" as being the main action on the move from symbolic to submicro level. We interpret H_2 as two atoms of hydrogen bonded to form a molecule. On the other hand, from a macro angle, we think on the substance hydrogen, "materializing" the representation in something closer to the experiential world.

Let's consider, for instance, the general concept of chemical reaction and analyze the major purposes of moving between the levels (Figure 2.11):

- **macro to submicro** - explain what happens during the chemical transformation through the rearrangement of the atoms, ionic change …
- **symbolic to submicro** - interpret a chemical equation as the rearrangement of the atoms between reactants and products of the reaction;

- **submicro to symbolic** – writing chemical equations, representing Lewis diagrams…
- **macro to symbolic** – communicate events in chemical language, express proportions and relations;
- **submicro to macro** - apply the model behind chemical reaction to real systems, predicting the formation or planning how to produce new substances;
- **symbolic to macro** - materialize the chemical formulas, proportions and expressions into physical substances and their macro properties, determining quantities like mass.

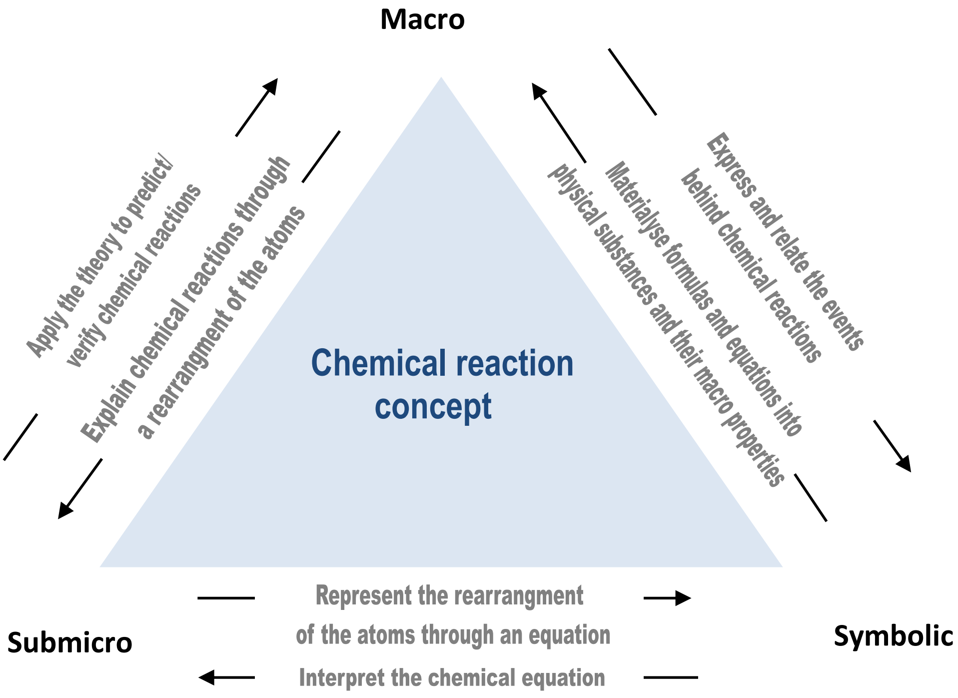


Figure 2-11 Relations between the macro, submicro and symbolic vertices forthe concept of chemical reaction.

About the human element, included by some of the authors reflecting on the triplet of chemistry (Christensson & Sjöström, 2014; Mahafy, 2004; Talanquer, 2011), we do not "physically" include it in our scheme of the chemistry knowledge space. Agreeing with Talanquer (2011), we think that more than being a fourth level, the presence of the human element is implicit on the approach in which the other three levels can be introduced, explored, and discussed. In the specific case of our expansion the human element controls the composition of the "mixture" of the three levels made according to the purposes, beliefs, motivations or background of the person working in / with chemistry. This issue will be discussed in chapter 3 from a pedagogical perspective, analyzing the consequences of teaching chemistry in the middle, edges or vertices of the triangle.

Our expansion of the triplet of chemistry mimics a ternary plot used to represent the quantitative composition of a mixture of three components. In this kind of graph each position inside the equilateral triangle corresponds to a certain ratio of the substances. We do not intend to reach so far in quantifying macro, micro and symbolic character of concepts, models, knowledge or processes involved in chemistry, but we can use the reasoning underlying a ternary plot to show that next to the vertices there is an absolute majority of the character from one of the levels and next to the centre there are only relative majorities.

We propose an expansion to Johnstone's (1991) triplet relationship, giving meaning to the inner triangular area. Each point inside the triangle represents a particular combination of macro, micro and symbolic character (mimic with a ternary plot used to represent the quantitative composition of a mixture of three components). In this framework instead of vertices of absolute macro, micro or symbolic nature, we have zones of dominant macro, micro or symbolic character (Figures 2.9 and 2.10).

Discussion about the pedagogical implications from this triple nature of chemistry will be part of Chapter 3, where the expansion presented in figure 2.9 will be used as base to discuss the teaching of CE.

2.2. Chemical Equilibrium: specific nature of the concept

"The meeting of two personalities
is like the contact of two chemical substances:
if there is any reaction, both are transformed.

Carl Jung, Swiss psychiatrist (1875 - 1961)

For the explanation of phenomena such as the formation of stalactites and stalagmites, the dynamics of the aquatic environment or acid rain, chemistry essentially uses a model based on thermodynamics and chemical kinetics: the Chemical Equilibrium (Atkins, 1998; Chang, 2005; Van Driel & Gräber, 2002). As several themes of the chemistry curriculum, Chemical Equilibrium has a specific nature that should be considered (Tyson et al., 1999). Three key basic ideas are recognized in the concept of Chemical Equilibrium: incomplete reaction, reversibility and dynamics (Quílez, 2004). Later, Quílez (2008) refers a fourth idea to be considered: equilibrium constant. When a chemical reaction evolves to a state of chemical equilibrium there is no tendency for the quantities of reactants and products to change. This concept is closely connected to the idea of incomplete reaction (a chemical reaction on which neither of the reactants is entirely consumed) and grounded on the fact that a reaction can take place in both directions (reversibility). The state of chemical equilibrium is characterised by a quantity, the equilibrium constant (Quílez, 2008). These concepts are explained at a molecular level, based on the idea of dynamics (Quílez, 2008). Both mathematical reasoning and molecular dynamics are key theoretical tools in the explanation of equilibrium reactions (Quílez, 2008). Thus, CE (Chemical Equilibrium) proper represents the specific nature of chemistry, involving the different levels from Johnstone' triangle (macroscopic, submicroscopic and symbolic).

CE includes multiple factors and variables, the understanding of microscopic models, symbolic language, quantitative and qualitative knowledge and is strongly related to the domain of other themes (Fonseca, 2006). Chemical equilibrium is an integrating and unifying concept because it requires connections from several domains of chemistry, obliterating the distinction between varied ranges of chemical phenomena often taught independently (Ganaras et al., 2008). This concept not only connects several previous concepts but also involves reorganizing a whole lot of descriptions that were previously expressed in other terms (chemical reaction, change of state, solubility and limit of solubility, etc.) (Ganaras et al., 2008). So, Chemical Equilibrium structures many basic chemistry concepts, being a central complex concept in the chemistry curriculum, both in secondary education as well as in higher education (Ganaras et al., 2008; Quílez, 2009).

First, we will take a look on the history around the concept of chemical reaction, which lies behind the idea of Chemical Equilibrium.

The first explanations for chemical reactivity are associated to the concept of affinity. The first idea of affinity, as a term expressing the tendency of substances to react, was introduced by Albertus Magnus in 1250 (Quílez, 2004; Thims, 2007; Partington, 1937). This concept stated that the greater the affinity (resemblance, similarity or relationship) between two chemicals, the greater is the tendency of these substances to react (Quílez, 2004; Weller, 1999). Boyle and Newton, among others, developed the idea of elective affinity (Partington, 1937; Thims, 2007). Boyle intended to liberate the idea of affinity from a certain anthropomorphism used in the explanation of the attraction between substances, pursuing mechanical laws to regulate chemical reactivity (Thims, 2007). Newton tried to address a theoretical explanation about some substances reacting with others, considering that in chemistry there would be forces similar to the gravitational ones manifesting only at very short distances. Newton introduced a mechanical view for chemistry (Quílez, 2004) and is considered to be one of the major developers of the theory of affinity (Thims, 2007). This theory is seen as one of the first branches studied in Physical Chemistry (Partington, 1937).

The first steps on the use of representations for chemical reaction is attributed to Jean Beguin, who drew the first diagram of a chemical reaction in his book from 1615 (Crosland, 1959; Lakshminarayanan, 2010). He made the first-ever chemical equation or rudimentary reaction diagram (Figure 2.12), detailing the reaction of corrosive sublimate ($HgCl_2$) with Antimony Sulphide (Sb_2S_3) (Crosland, 1959; Lakshminarayanan, 2010):

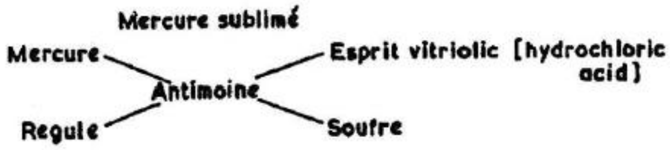


Figure 2-12 First "chemical equation" or rudimentary reaction diagram – after Lakshminarayanan, 2010; Crosland, 1959.

The earliest affinity table was published by E.F. Geoffroy in 1718 (Figure 2.13) (Grapí, 2011; Quílez, 2009) based on the "Quest 31" from the "Opticks" book of Newton (Thims, 2007). In this table, composed by sixteen columns, there was the traditional symbol of a substance (or a group of substances to which it refers) at the head of each column. Below there were the symbols for the substances with which it reacts, arranged in order of their affinity for it (Quílez, 2009; Thims, 2007). The table was organized so that each substance will displace from combination any of those lower down the column (Quílez, 2009). Geoffroy preferred the use of the term "relation among substances" to describe the content of its table (Thims, 2007).

Many scientists contributed to the development of affinity tables (Quílez, 2009). The Swedish chemist T. O. Bergman made the most extensive studies of displacement reactions. (Quílez, 2009), elaborating several affinity between 1775 and 1783 (Weller, 1999; Grapí, 2011). Bergman considered that all chemical reactions were complete and took place only in one direction. He was aware of other factors that also affected chemical reactions, namely that some reactions required an excess of reactant to proceed to completion (Partington, 1937), but he did not believe that any influence other than heat could mask the forces of affinities (Quílez, 2009). According to Bergman's theory when a substance A reacts with a compound BC, the substance B is replaced by A, and the new compound AC is produced.

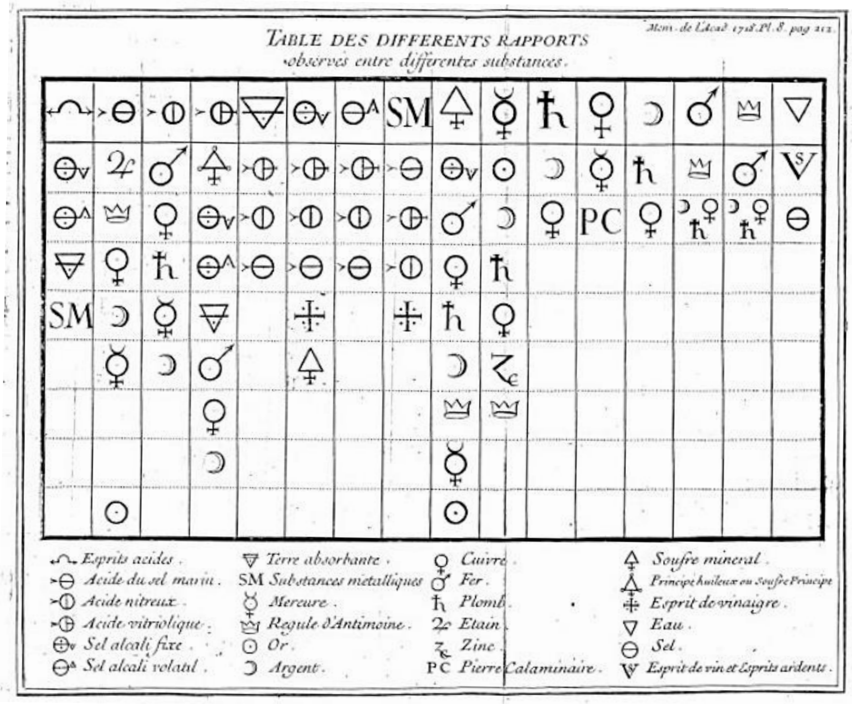


Figure 2-13 Geoffroy's Table of the different relations observed in chemistry between different substances (1718) - after Grapí, 2011

Cullen began to use Geoffroy's original table in 1757 (Thims, 2007). He was the first to represent a chemical equation of a displacement reaction using arrows, which he called "darts" (Figure 2.14). Cullen used this diagram in order to facilitate the explanation of chemical affinity effects to his students (Thims, 2007). A diagonal arrow represented affinity tendency and the brackets were used to represent the initial bond.

Figure 2-14 Cullen diagram of a single and double displacement reaction – adapted from Thims, 2007.

Cullen's single displacement diagram presented above, used the symbols from Geoffroy's original affinity table. Bergman, who also used diagrams, attributed letters to the species when reasoning about replacement reactions on the base of elective affinities (Thims, 2007). On Figure 2.15 we present a visual scheme, illustrating the first approach (with a conceptual grounding) used to represent a chemical equation, in a style that we will adopt along this section to illustrate the evolution on the schematization of chemical reactions.

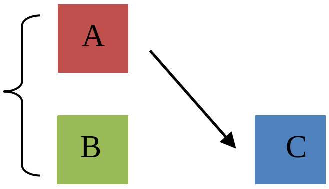


Figure 2-15– Diagram of a chemical reaction based on the elective affinity theory.

As it will be analysed to the end of this section, the evolution on the representation of chemical reactions reflects the evolution in their conceptual understanding. Figure 2.16 illustrates the knowledge about chemical reactions in the end of eighteen century which corresponds to the interpretation of Cullen's diagram.

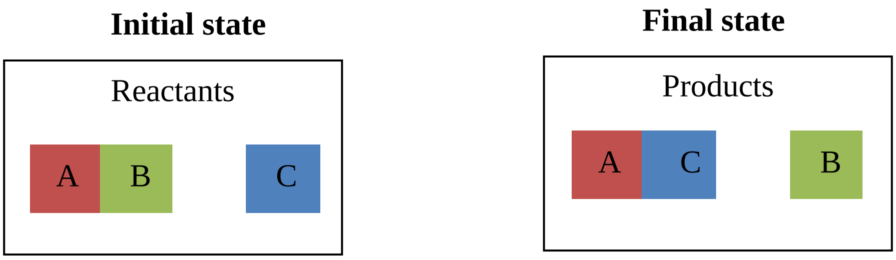


Figure 2-16 Interpretation of the diagram from figure 2.13, reflecting the knowledge about chemical reactivity at the end of eighteen century.

Some inherent difficulties concerning the theory of affinity presented themselves along the way. Boyle, in 1674, made references to the fact that "quantity can compensate strength". Bergman referred to the effect on the quantity of reactant. Cullen and Bergmen made references to the heat effect (Partington, 1937; Thims, 2007). In 1782 Lavoisier pointed the importance of drawing affinity tables for each degree of the thermometer (Thims, 2007). Nevertheless at the end of the 18th century, the concept of affinity was consolidated as a constant property of the substances that manifested itself in an elective way (Quílez, 2004). “If two substances combined, they were thought to have a selective or "elective" affinity for each other.” (Weller, 1999). Since elective affinity was constant for each combination of substances, at the end of the 18th century, reactions were understood to occur only in one direction and proceed to completion (Grapí, 2011), as can be interpreted from figure 2.16.

Based on the affinity tables, some figurative diagrams were published in books from the end of eighteen century, intended to facilitate the use of the elective affinities to interpret chemical double decompositions (Figure 2.17) (Grapí, 2011). Fourcroy’s chemistry textbooks diagram was one of the first attempts to use simbology in the treatment of chemical reactions preceding chemical equations. So, the earliest precursor of the modem chemical equation is the affinity diagram (Jensen, 2005). Since they contained the names of substances according to the new nomenclature, they were also appropriate for the introduction of the new nomenclature and for the diffusion of the new antiphlogistic chemistry (Grapí, 2011).

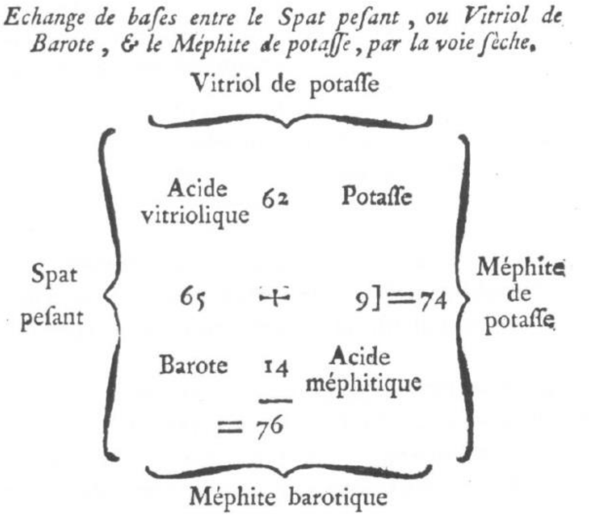


Figure 2-17 Fourcroy’s chemistry textbooks scheme based on elective affinities to explain double dissociations (Grapí, 2011).

These diagrams used to have hypothetical numerical affinity, but there wasn´t by the time yet any quantitative understanding of chemical reactions in terms of stoichiometry – relative proportions in which reactants combine. Even the law of conservation of mass was relatively recent – attributed to Lavoisier in 1774. So, by the end of eighteen century, the knowledge about chemical reactivity had a purely qualitative character – it was possible to predict the occurrence of a reaction according to affinities, representing the substances present in the initial and in the final state. Chemical reversibility was thus theoretically forbidden (Grapí, 2011).

The quotation included in the beginning of this chapter establishes an analogy between the meeting of two personalities and the contact of two chemical substances, stating that if there is a reaction, both are transformed. But would it be possible to reverse the transformation in the personalities? In chemistry, Bertholet found that it is possible to reverse the reaction!

As referred above, several difficulties were verified with the affinities theory. From the practice of chemistry arose several actual instances of chemical reversibility, those remained as persistent anomalies until the end of eighteenth century (Grapí, 2011). Bertholet was the first to clearly point the effect of mass (Partington, 1937). Napoleon Bonaparte asked Berthollet to organize a "Committee on the Arts and Sciences" to accompany the army during an expedition to Egypt in 1798 (Lower, 2001; Weller, 1999). Once in Egypt, Bertholet verified that some lakes were bordered by a thick crust of natron (hydrated sodium carbonate) (Quílez, 2004; Weller, 1999). Bertholet concluded that the sodium carbonate should have been formed by the action of salt water on limestone. Berthollet was already familiar with the opposite process: adding solid Na_2CO_3 to a solution of $CaCl_2$ producing a precipitate of $CaCO_3$. From laboratory experience, Bertholet believed that this process was irreversible and this reaction appeared to go essentially to completion (Treptow, 1980; Weller, 1999):

$$Na_2CO_3\ (cr) + CaCl_2\ (aq) \rightleftharpoons CaCO_3\ (cr) + 2\ NaCl\ (aq) \tag{1}$$

In the Natron Lakes, where salt water and underlying limestone were in contact, this reaction seemed to be partially reversed (Weller, 1999). The reaction in the lake was the inverse of the reaction predicted by the theory of elective affinities, putting in question the accepted paradigm.

These observations led Bertholet, who initially adhered to the paradigm of elective affinities (Quílez, 2004), to question if a reaction could only take place in one direction. “He correctly inferred that chemical reactivity depends not only on the "elective affinities" of the reactants, but also on the relative masses of reactants and products.” (Weller, 1999).

Initially the occurrence of a chemical reaction was explained according to the affinity between substances, which was considered to be a constant, determining that once a reaction begins it would always be complete. Bertholet was the first to argue that certain chemical reactions could be reversible, depending on the relative masses of reactants and products.

Berthollet reached this conclusion reflecting on the effect of the great quantities of sodium chloride and calcium carbonate present, the continuous removal of sodium carbonate that formed a crust around the edges of the lake and the deliquescence of calcium chloride, which seeped into the ground (Quílez, 2004). So, the relative quantities of the substances intervening in the transformation appeared to have an effect on the progression of this reaction. “Later, Berthollet was able to find other instances where unexpected reactions could be observed.” (Quílez, 2009) Bertholet seemed to have a notion of the effect of an excess of one of the substances involved the reaction: “excess of quantity of the body whose affinity is the weaker, compensates for the weakness of affinity” (Bertholet cited in Weller, 1999). That is, if two substances were competing to combine with a third substance for which they had unequal affinities, a relative large quantity of the substance with weaker affinity might exert a force that could surpass the force of the substance with greater affinity. Eventually, Berthollet considered that any displacement reaction was never complete but that there was an equilibrium state between opposite affinity forces. (Quílez, 2004; 2009).

Berthollet adhered to the Newtonian ideas, interpreting the occurrence of a chemical reaction based on a kind of gravitational force dependent on the affinity and the quantitative proportion of the substances. “Thus, any displacement reaction was never complete: there was an equilibrium state between opposite affinity forces.” (Quílez, 2004). The leading concept was now “chemical action”, understood as the tendency between two different substances to form a new combination, exerted according to both their relative affinity and their proportional amounts. (Grapí, 2011; Quílez, 2004).

Berthollet built his interpretation of chemical reactivity around the laws of chemical action (Grapí, 2011):

- first law (the partition effect) - when a substance acts on a compound, the subject of the combination is shared between the other two substances, depending on their affinities and their weight proportion.

- second law (the mass quantity effect) - the quantity of a substance could substitute the effect of the affinity to produce the same degree of saturation.

Bertholet's conclusions constituted the first theoretical qualitative presentation of reversibility and incomplete reaction and the first account for the development of the equilibrium concept in chemical reactions. Berthollet objected to the absoluteness of elective affinity, conveying that the mass of the reactants could reverse the reaction predicted by the scale of relative affinities (Quílez, 2009). Summarizing, according to Bertholet's reinterpretation:

- some chemical reactions were reversible, occurring in both directions;

- chemical reactions do not always proceed to completion, instead a reaction can evolve to a "state of equilibrium" where reactants coexist with products;

- the relative amounts of the substances participating in the reaction and their relative affinities determine the direction in which the reaction occurs and the final composition of the mixture;

- the excess of one of the reactants can force the consumption of the other reactant due to the displacement of the reaction towards the products.

It is possible to redraw the schemes from figures 2.13 and 2.14, illustrating the reconceptualization made in the idea of chemical reaction in order to include reversibility

(Figure 2.18), incomplete reaction (Figure 2.19), "mass effect" (Figure 2.19) and state of equilibrium (Figure 2.19).

Figure 2-18 Diagram of a chemical reaction considering the possibility of reversible reactions.

Figures 2.18 and 2.19 illustrate Bertholet's idea that producing AC from the contact between AB and C is not an exclusive process. When exposing AC to B, A will divide itself between B and C in proportion to their affinity and their quantity (Quílez, 2009).

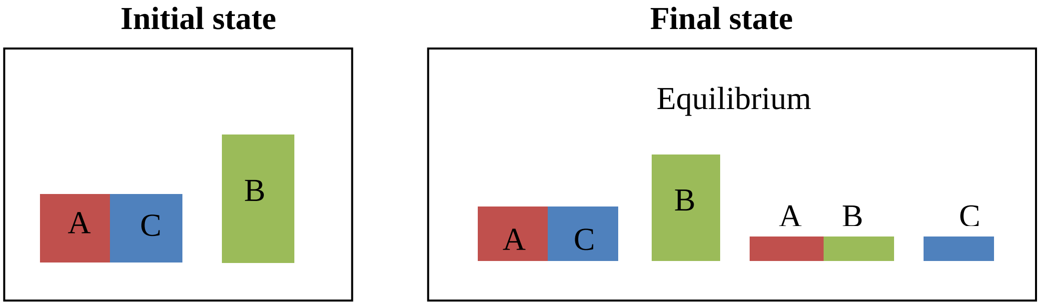


Figure 2-19 The knowledge about chemical reactivity after Bertholet's reconceptualization

Berthollet's mass action ideas were well ahead of his time (Welller, 1999) and allowed the acceptance of chemical reactions as reversible and incomplete processes. Also, Bertholet developed the first ideas on the equilibrium state, in a manner analogous to mechanics: static view (Quílez, 2004; Macdonald, 1976). Although, an initial idea of a ratio between opposite affinity forces was referred, "chemical equilibrium" was not given a precise definition by that time (Quílez, 2004).

Equilibrium according to Bertholet – a static state to which chemical reactions could evolve, resulting from the balance of opposite forces related to the relative affinities and the amounts of the substances. Reactants and products coexist in equilibrium state.

Berthollet considered the formation of compounds in variable proportions (Grapí, 2011, Quílez, 2004), This incursion of Bertholet trough "stoichiometry" was inconsistent with Dalton's new atomic theory and the principle of definite proportions established by Proust. (Quílez 2004). Berthollet's belief was contrary to that of fixed proportions of combination that Proust claimed to have proved. Proust's point of view proved to be more successful and was finally adopted by chemists (Grapí, 2011). So, Bertholet wasn't able to quantify the "forces" determining the evolution of reactions.

Berthollet's concepts were qualitative in nature, and there was no quantitative development for many decades (Weller, 1999; Treptow, 1980), until both mathematical reasoning and molecular dynamics became key theoretical tools in the explanation of equilibrium reactions. (Quílez, 2004) The fact that atomic theory was in "exponential" development is one of the reasons pointed for the delay in the new developments on the understanding of chemical reactions: "the chemists of the time were primarily concerned with the problems of chemical elements and their atomic weights" (Quílez, 2009). Other possible contributing factor was the slow realization that quantitative physical laws had important applications in chemistry (Weller, 1999). "Physical chemistry was explicitly recognized as a new subdiscipline only in the latter half of the nineteenth century" (Weller, 1999) When affinity was back to attract the attention of chemists, it could evolve in the light of new kinetic and thermodynamic ideas (Quílez, 2009).

In the meantime, the appearance of linear chemical equations and the accompanying use of the equal sign to separate the reactants from the products began in the late 1840s (Jensen, 2005). “It has been argued that this switch from diagrams to linear equations reflects a change in emphasis from the inequality of Newtonian forces of affinity to the conservation of Daltonian atomic and/or equivalent weights in chemical reactions” (Jensen, 2005). Curiously, Lavoisier was the first to represent a chemical reaction with the equal sign to show the algebraic character of the equation that could be used to calculate proportions (Alvarez, 2011). Nevertheless, linear equations only became relevantly used in the middle of 19th century, probably because the law of conservation of matter from Lavoisier could now be applied in micro scale referring to the conservation of the number of atoms. So, continuing the “style” used in the diagrams from figures 2.15, 2.16, 2.18 and 2.19, we use now circles as an effort to represent atoms according to Dalton’s model. This kind of representation shows the conservation of matter at submicro scale (Figure 2.20).

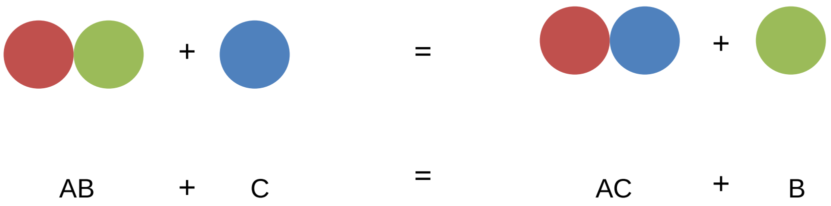


Figure 2-20 Visual representation of submicro events in a chemical reaction according to the first chemical linear equations used in the middle of 19th century.

From the middle of the 19th century there were sequential efforts in explaining reversible reactions and chemical equilibrium, alternating between kinetical and thermodynamical approaches.

Atomic scale considerations started to take part and inspire the explanations. In 1850, Williamson was the first scientist to propose a submicroscopic model in order to explain the state of equilibrium. He considered that equilibrium results from two simultaneous operations: two reactions run simultaneously, each in opposite directions, in a way that the amount of all the substances involved remains constant (Macdonald, 1976).

From the middle of the 19th century atomic theory started to take place in chemical reactivity explanations. The occurrence of simultaneous opposite processes during equilibrium state was proposed to justify the maintenance of the amount of all the substances involved. This might be considered the first glance on the concept of dynamic equilibrium, which became gradually clear in face of later contributions.

Quantitative formulations concerning the rate of reactions were also beginning to develop. In 1850 Ludwig Wilhelmy did publish the first quantitative measurements of the rate of a chemical reaction fitting it to a rate equation corresponding to a pseudo first-order irreversible reaction (Weller, 1999). This is often considered the birth of chemical kinetics (Quílez, 2009) Extensions of Wilhelmy's work to the kinetics of a reversible reaction did not occur for more than another decade — by Marcelin Berthelot and Saint-Gilles, among others (Weller, 1999): “Berthelot and Saint-Gilles had established that the amount of ester formed at any instant was proportional to the product of the amounts of the reacting substances (i.e. alcohol and acid) and inversely proportional to the volume. They also found that the reaction did not reach completion but progressively approached a limiting situation (i.e. equilibrium), where all four substances were present at the same time. Berthelot and Saint-Gilles gave a mathematical formulation of the phenomenon but they failed to take the reverse reaction between ester and water into consideration.” (Quílez, 2009).

From the middle of the 19th century the first quantitative efforts on describing equilibrium state also started to show up. In 1864, Guldberg and Waage formulated the law of mass action - a first approach to equilibrium constant. Nevertheless, in the first presentation of this expression, chemical equilibrium was still treated as a static balance of forces; the forces driving the forward reaction must be equal to the forces driving the reverse reaction. Only later it evolved in terms of kinetics.

Guldberg and Waage took into account mechanics as a paradigm and considered together the opposite forces in order to develop a mathematical theory of chemical affinity. Unlike Berthollet, Guldberg and Waage assumed that chemical forces were not proportional to the amounts of the substances involved in the reaction, but to the concentrations. For each substance, the concentration (they used the term active mass) had a power that they determined by experiment. For a generic reaction

$$P + Q = P' + Q' \tag{2}$$

designating p, q, p' and q' the concentration of these substances, Guldberg and Waage established the law of mass action in 1864, writing the equilibrium condition as (Quílez, 2009):

$$\alpha(p-x)^{a}(q-x)^{b} = \alpha'(p'+x)^{a'}(q'+x)^{b'} \qquad (3)$$

where p and q are the reactants initial concentrations; p’ and q’ are the products initial concentrations; α and α’ are proportion constants related to the balance of opposite forces; x is the amount of material that had to be converted during the approach of the “steady state” (equilibrium state) and a, b, a’ and b’ are exponents to be determined by experiment.

In the equilibrium, the forces driving the forward reaction must be equal to the forces driving the reverse reaction. “The above equation was indeed the first equation that approximates the mathematical expression of what we call nowadays equilibrium constant. But, we must notice that exponents were determined empirically (Van Driel and Gräber, 2002) and, thus, they bore no relationship to the stoichiometry (Quílez, 2009). In the early works of Guldberg and Waage, concerning the formulation of the law of mass action, the concept of chemical equilibrium was still treated mechanically as a balance of forces and there wasn’t yet the notion of dynamic equilibrium in this quantitative incursion. In later papers of the same year (1864), Guldberg and Waage argued in terms of the rate of the reactions in forward and reverse directions, associating each side of expression 3 to the rate of the reaction in the respective direction. For the rate of forward reaction (Quílez, 2009):

$$v = \frac{dx}{dt} = k(p-x)^{a}(q-x)^{b} \qquad (3)$$

where v is the velocity of reaction, x is the quantity transformed in the time t, and k a constant depending on the nature of the system, including the temperature.

Guldberg and Waage concluded that the rate of the net reaction was considered to be the difference of the two velocities (Quílez, 2009):

$$v_{\text{net}} = v_{\text{forward}} - v_{\text{reverse}} \qquad (4)$$

And, thus, they defined the equilibrium condition: $v_{\text{net}} = 0$. Nevertheless, initially Guldberg and Waage treated equilibrium in terms of forces so their approach was considered to have small evolution in terms of kinetics by several authors (Quílez, 2009). Their major contributes were considering the concentrations of the substances involved in the equilibrium system (instead of their amounts), taking into account the occurrence of a reverse reaction (Quílez, 2009) and the experimental proof that in an incomplete reaction a definite equilibrium is reached and can be approached from either direction (Macdonald, 1976).

In terms of kinetics, the quantitative formulation for equilibrium state is grounded on the equality between forward and reverse reaction rates:
At equilibrium:

$$v_{\text{forward}} = v_{\text{reverse}}$$

The work of Guldberg and Waage, written in Norwegian, only reached the knowledge of several scientists working in the field when they published an article in German in 1878. In this paper they included considerations of microscopic nature based on molecular kinetics, ideas emergent at the time in several other works from scientists like Van’t Hoff and Pflaunder (Quílez, 2009). Also, in 1878 there were already other contributions to the formulation of a mathematical expression for the equilibrium constant, like Horstmann for what concerns to gases (1873) and Van’t Hoff for esterification (1877) (Macdonald, 1976).

Based on Clausius’s ideas about the nature of heat, some authors tried to explain both physical and chemical processes in terms of molecular kinetics (Quílez, 2009). In 1857, Clausius explained the partial evaporation of liquids in closed systems based on the molecules’ kinetic energy. This was assumed as a dynamic equilibrium because it implied a state in which both evaporation and condensation simultaneously happened, exchanging equal number of molecules. So there is not a state of rest, but a state of simultaneous evaporation and condensation of equal magnitudes (Quílez, 2009). We owe to Clausius the idea that the heat of a body is related to the movement of its molecules. Ten years after Clausius' paper on the kinetic theory of evaporation, Pfaundler applied these previous physical ideas to develop a theory of chemical dissociation. Pfaundler was the first scientist who gave a correct account of partial dissociation, assuming that, at constant temperature and pressure, equal amounts of molecules decompose and unite by collision (Quílez, 2009). This assumption was based on the theoretical background of the mechanical theory of heat. That is, that explanation required that not all molecules were in the same state of motion at a given temperature, for only a small number of collisions were effective to produce chemical reaction (Quílez, 2009). Pfaundler applied his ideas to chemical equilibrium and to the law of mass action. His explanations, in terms of motion of individual molecules, provided better explanation than previous Williamson's idea that there was a continuous exchange of elements in a molecular aggregate (Quílez, 2009). Pfaundler's explanation is considered the most important qualitative kinetic-molecular rationale, anticipating much of the conceptual basis of modern chemical kinetics (Jensen, 2009).

Van't Hoff, in 1884 published his research on chemical kinetics and defended that the laws that rule the relative quantities in equilibrium, under given conditions of volume and temperature, can be approached experimentally and theoretically from two points of departure, namely thermodynamics and the kinetic theory (Quílez, 2009). Van't Hoff rather than worrying about the end product at the equilibrium state turned his attention to how the equilibrium state was reached, focusing on the dynamics of reversible reactions (Quílez, 2009). "Before 1850 it was thought that when a chemical system is at equilibrium all reaction has ceased." (Quílez, 2009). Based on previous explanations given by Williamson (1851), and mainly by Pfaundler (1867), Van't Hoff's starting point was considering chemical equilibrium as a result of two changes taking place with the same velocity in opposite directions (Quílez, 2009).

For a reaction of the type $A \rightleftarrows 2\,B$, Van't Hoff derived the expression:

$$k_1 C_A = k_2 C_B^2 \qquad (5)$$

where C represents concentration of the species A and B and k is the velocity constant for the forward and reverse reactions. This can be generally presented as:

$$k_1 C_1^{n_1} = k_2 C_2^{n_2} \tag{6}$$

Where n_1 and n_2 represented, according to Van't Hoff the "number of molecules in each of the systems that take part in reaction" (Quílez, 2009). The expression combined the mathematical description from Guldberg and Waage with the submicro explanation of Pfaundler in terms of molecular kinetics, providing the old law of mass action an explanatory and predictive character that wasn't yet exposed. The constant of equilibrium (K) could now be clearly expressed in terms of the ratio between velocity constants of the forward and reverse reactions or according to the ratio between equilibrium concentrations elevated to the respective stoichiometric number:

$$\frac{C_2^{n_2}}{C_1^{n_1}} = \frac{k_1}{k_2} = K \tag{7}$$

The importance of Van't Hoff as the spreader of dynamic equilibrium is reflected on the introduction of a new symbol for chemical reactions in 1884, that he used in his publication (Van't Hoff, 1901). So, although the concept of chemical equilibrium was introduced by Berthollet as early as 1801 and was given a kinetic rationale by Guldberg and Waage as early as 1864, it was not until the end of the 19th century that this concept impacted on the symbolism used in the writing of chemical equations." (Jensen, 2005).

Van't Hoff was the responsible for the introduction of double arrows to indicate the presence of a reversible equilibrium (Jensen, 2005; Quílez, 2009) (Figure 2.21). The concept of dynamic equilibrium was incorporated on the formalism of chemical equation (Alvarez, 2011) So, the change from equal sign to arrows doesn't represent just a choice of symbol but constitutes a conceptual step forward (Alvarez, 2011) It is curious to notice that the single arrow appeared after the double arrow and gradually became disseminated in chemistry text books (Alvarez, 2011).

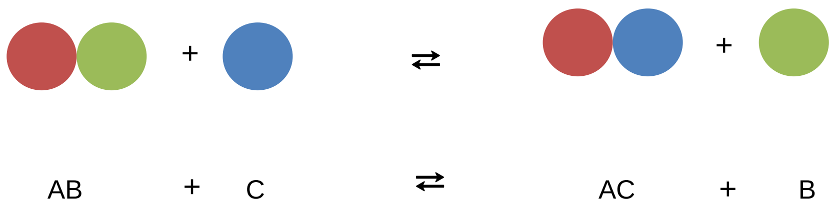


Figure 2-21 Visual representation of chemical equations according to the symbolism at the end of 19th century.

The double arrow in the chemical equations reflect once again an evolution in the conceptualization on the phenomena of chemical change: equilibrium is no longer seen as mechanical static balance between opposite forces but as a dynamic equilibrium resulting from two opposite chemical processes occurring simultaneously. A more elaborate symbolism was proposed by Marshall in 1902 which included the use of the currently favoured double barb for equilibrium reactions (Figure 2.22). (Jensen, 2005; Lakshminarayanan, 2010). Marshall's justification was that the common arrows were used in organic chemistry with a different meaning from that intended in a chemical equation (Alvarez, 2011).

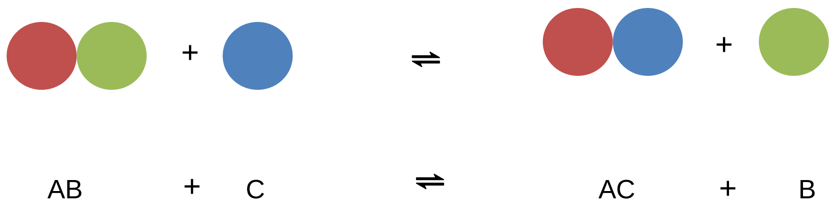


Figure 2-22 Visual representation of chemical equations according to the symbolism proposed at the beginning of 20th century.

Figure 2.23 intends to point the simultaneity of opposite processes at equal rate, exposing the dynamic character of equilibrium state.

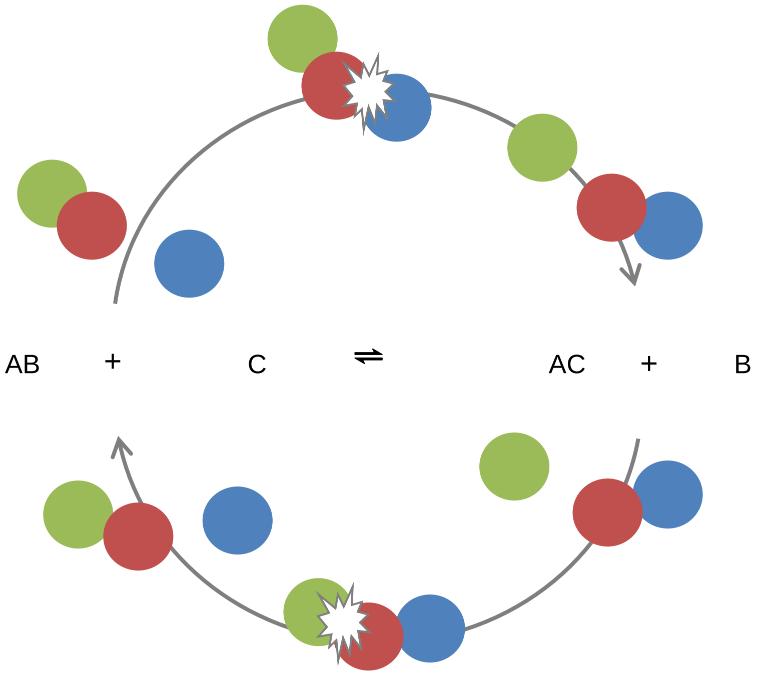


Figure 2-23 Visual representation of dynamic equilibrium

As seen above, from the second half of 19th century there were gradual advances in the explanation of chemical equilibrium, grounded mainly on microscopic and kinetic considerations. The consolidation of the concept of dynamic equilibrium justifies another evolution in our schematization along this section: Figure 2.24 is the first to include a multiparticle representation of the progression to equilibrium state. This interpretation requires the use of ideas such as the continuous movement of molecules, effective collisions and equality in the rates of forward and reverse reaction during equilibrium, resulting in the maintenance of concentrations.

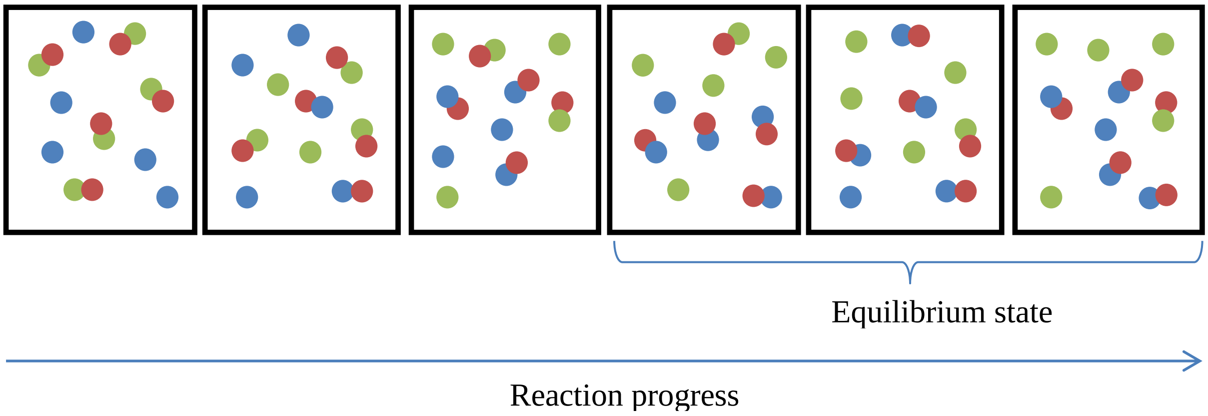


Figure 2-24 Multiparticle microscopic representation of a reaction's progression to equilibrium.

Although there was a clearer idea of dynamic chemical equilibrium based on a kinetic approach, both from qualitative and quantitative perspectives after the works of Pfaundler and Van't Hoff, the phenomenon of chemical reactivity, namely the motives beyond affinity, was still a mystery (Macdonald, 1976). Berthollet has regarded the force as similar to gravitational force. Berthelot (1827-1907) and Thomsen (1826-1908) considered the heat evolved by a reaction to be a measure of the driving force but reactions also occurred which were endothermic (Macdonald, 1976). The development of thermodynamics and the use of its principles in chemistry came to shine a light over this issue.

Van't Hoff presented an approach that combined the mathematical description from Guldberg and Waage (law of mass action) with the submicro explanation of Pfaundler in terms of molecular kinetics. He clearly expressed the constant of equilibrium in terms of the ratio between velocity constants of the forward (f) and reverse (r) reactions or according to the ratio between equilibrium concentrations elevated to the respective stoichiometric number.

For a reaction of the type

$$m\mathrm{A} + n\mathrm{B} \rightleftharpoons q\mathrm{C} + r\mathrm{D}$$

$$K_c = \frac{k_f}{k_r} = \frac{[\mathrm{C}]^q.[\mathrm{D}]^r}{[\mathrm{A}]^m.[\mathrm{B}]^n}$$

Nevertheless, the motives behind chemical reactivity were still misty, which appealed to an incursion trough thermodynamics.

In the thermodynamic field, the phenomenon of Chemical Equilibrium was first associated with the concept of entropy, by the work of Horstmann. Horstmann gave an explanation of dissociation, using not a kinetic theory like Pfaundler, but the second law of thermodynamics[1]. "Horstmann concluded that, in general, the degree of dissociation depends on the entropy or on factors that influence the entropy (temperature, pressure, quantities of reactants)" (Quílez, 2009).

Entropy is a system property usually associated with the amount of disorder (Reger et al., 1997). Nevertheless, the first definitions of entropy were mostly related to the operation of engines and came up by the interest of physicists and engineers in describing and quantifying the work that could be done from a hot system (in order to move a turbine for instance). Thus, in this context, entropy is usually associated with the part of the total energy of a system that cannot be converted into work. In other words, entropy represents the unavailability of a system's thermal energy for conversion into mechanical work.

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[1] The Second Law of Thermodynamics states that the Entropy of the entire Universe, as an isolated system, will always increase over time. According to the second law of thermodynamics, any spontaneous process must increase the entropy in the universe:

$$\Delta S\text{universe} = \Delta S\text{system} + \Delta S\text{surroundings} > 0$$

In 1873, Horstmann gave the first, although incomplete thermodynamic explanation of the Guldberg-Waage law of mass action proposed in 1864: found that in dissociation processes the equilibrium state is reached if the entropy of the system is at a maximum (Van Driel & Gräber, 2002; Quílez, 2009). Today, the contribution of Horstmann is recognised as pioneer works in chemical thermodynamics, but they were neither well known nor fully recognized by his contemporaries (Quílez, 2009). Horstmann's paper from 1873, entitled Theorie der Dissociation, took an entirely new approach at the time, based on an explicit application of Clausius' new entropy function[2] (Jensen, 2009).

Horstmann, argued that a system is in Chemical Equilibrium when its entropy has a maximum value (Van Driel & Gräber, 2002), associating that the system tends to a more stable situation. Horstmann formulated the equilibrium condition for dissociation as a direct function of having maximized the change in the total entropy (dS) of the isolated system with respect to the degree of reaction or dissociation (dx):

$$(\mathrm{d}S/\mathrm{d}x) = 0 \tag{8}$$

---

[2] Clausius presented an equation for the entropy in a reversible cyclic process in the form of:

$$\int \frac{dQ}{T} = S - S_0$$

where S is the entropy of the final condition of a body, and S_0 denotes entropy of the initial condition of the body (Howard, 2001), where T is the absolute temperature of the system and Q represents transfer of heat into that system (if heat is transferred out the sign would be reversed giving a decrease in entropy of the system). This expression is usually rewritten as

$$\mathrm{d}S = \mathrm{d}Q_{rev} / T$$

where Q is the heat exchanged by the system in the reversible process and T is the absolute temperature of the system (in the place were heat is exchanged). This means that, at reversible processes, the variation in entropy is measured according to the overall change in heat transfer at a particular temperature.

A new insight on the idea of entropy came by when Clausius presented a function composed of two terms by writing the following equation:

$$\mathrm{d}Q / T = \mathrm{d}H / T + \mathrm{d}Z / T$$

where $\underline{H}$ is the quantity of heat contained in a body, dH is the change of this quantity, and Z is "disgregation" (Howard, 2001). This latter quantity was first introduced by Clausius in 1862 to express the variation in the degree of molecular aggregation. (Jensen, 2009). Clausius also uses two sentences to resume succinctly the conclusions from his work:

1. The energy of the universe is constant.
2. The entropy of the universe tends to a maximum.

Horstmann explained his mathematical expression for the equilibrium condition: “A reaction, whatever its type, can only begin and proceed so long as collective sum of the various entropy changes contributed by the individual processes increases, since, as we know, the total entropy cannot decrease. The reaction must therefore stop at the very instance when the decreases become larger than the increases, i.e. at that point when the total increase becomes zero.” (Horstmann, 1873) in which the total entropy production was given by the equation:

$$S = (Qx)/T + Z \qquad (9)$$

where Q is the heat of reaction per mole, T is the absolute temperature and Z is the change in the “disgregation” of chemical reactants and products (Jensen, 2009). Horstmann’s work led to the incorporation of Clausius’ rationale in a particularly fruitful thermodynamic treatment of chemical systems (Jensen, 2009; Thims, 2007). Horstmann proceeded to a case by case analysis (Jensen, 2009). Horstmann’s specific results at equilibrium can be generalized using the master equation:

$$(\mathrm{d}S/\mathrm{d}x) = q/T - AR\ \ln K + C = 0 \qquad (10)$$

where q is the equilibrium value of Qx, A is the mechanical equivalent of heat, R is the universal gas constant, C is the change in the disgregation of the various reactants and products when in their standard states, and K is the equilibrium constant, although Horstmann himself never took the final step of subsuming concentration and/or pressure ratios at equilibrium under a single generalized symbol K (Jensen, 2009).

Horstmann was the pioneer in the thermodynamic treatment of equilibrium. He associated equilibrium conditions to a maximum value of total entropy. Entropy is a system property usually considered to be connected to the level of disorder. The reaction reaches equilibrium when the total increase in entropy becomes null because entropy has already reached a maximum possible value.

In the case of a non-isolated system, it is the entropy of the universe that must be taken into consideration. The system spontaneously evolves into a state because the entropy of the universe increases, namely, the variation of entropy of the universe is positive. (Reger et al., 1997). The reaction reaches equilibrium at that point when the total increase becomes zero.

Quantitative formulations of chemical equilibrium based on energy considerations were derived later by Van't Hoff and Gibbs (Van Driel & Gräber, 2002).

Van’t Hoff (1884), already referred in the context of kinetics, also developed a thermodynamic approach. In 1884, in his studies on chemical dynamics, he stated that the maximum work available from the operation of a chemical process was a measure of the chemical affinity (Macdonald, 1976). Van’t Hoff extended Horstmann’s equation to express the variation of the equilibrium constant with temperature, this work was recognized with a noble prize.

$$\frac{d\log K}{dT} = \frac{q}{2T^2} \tag{11}$$

The above equation from Van’t Hoff [3], expressing the work of affinity, is equivalent to the equation we write today, reason why this scientist is considered responsible for most of the concepts and relationships that are in current use in the current model of chemical equilibrium. (Quílez, 2009).

The maximum work of Van’t Hoff was replaced by “free energy”, a term coined by Helmholtz and given the symbol *G* in honor of Gibbs: a measure of the amount of energy available to do work in an isothermal and isobaric (constant temperature and pressure) thermodynamic system. A system in dynamic chemical equilibrium was recognised as a system of minimum free energy in which forward and reverse reactions proceed at equal rate. This is the modern interpretation (Macdonald, 1976). In modern terms we use “free

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[3] Also expression 11 is inspired in the Clausius-Clapeyron theorem, an expression to describe phase transition of a substance, which can be written as:

$$\frac{dln\, p}{dT} = \frac{Q}{RT^2}$$

were p represents vapor pressure, Q is the latent heat, R the gases constant and T is the temperature.

energy” to measure the affinity. The equation we use today was presented by Gibbs in a 1876 paper, applying the principles of thermodynamics to chemical equilibrium. He first named it as available energy, and later became known as free energy. This expression is used at constant pressure and temperature.

$$\Delta_r G = \Delta_r G^\circ + RT \ln Q \tag{12}$$

where $\Delta_r G$ is Gibbs energy for the reaction, $\Delta_r G^\circ$ is the standard Gibbs energy for the reaction, R is the perfect gases constant, T is the temperature and Q is the reaction quotient.

The condition for Equilibrium is the minimization of Gibbs’s free energy. So, at equilibrium: $\Delta_r G = 0$ and $Q = K$ and the equation is reduced to:

$$\Delta_r G^\circ = -RT \ln K \tag{13}$$

Writing the equation in order of the equilibrium constant you obtain:

$$K = \exp^{\left(-\frac{\Delta_r G^0}{RT}\right)} \tag{14}$$

The maximization of the Universe’s entropy as the equilibrium condition was reformulated by Gibbs: chemical equilibrium is now recognized as a system of minimum free energy (a measure of the amount of energy available to do work at constant temperature and pressure) in which forward and reverse reactions proceed at equal rate. Equilibrium condition is therefore the minimization of Gibbs free energy.

From Gibbs free energy definition, we can write:

$$G = H - TS \tag{15}$$

where H is the enthalpy[4] of the system, T *is* the temperature and S *is* the entropy of the system. From the above exposed, we can state that for a system at constant pressure and temperature the reaction is spontaneous if $\Delta_r G < 0$. It turns out, therefore, that the system tends to evolve to a state in which energy is minimal. Thus, Gibbs energy should have its minimum value at equilibrium state. The more favourable combination for minimizing G implies an increase in entropy (positive ΔS) and a decrease in enthalpy (ΔH negative). The enthalpy variation of the system corresponds to the heat transferred under conditions of constant pressure (Atkins, 1998). Thus, when the system increases in disorder and loses heat the reaction is certainly spontaneous. However, for a process to evolve spontaneously, other conditions are possible, as long as they result in a negative value of $\Delta_r G$. The spontaneity of the reaction depends on the relative quantities involved in the following equation:

The more favorable combination for minimizing Gibbs energy implies an increase in entropy and a decrease in enthalpy. So, we can state that the spontaneity of a process is granted when the system increases in disorder and loses heat. If the system absorbs heat then it necessarily increases in disorder and if it decreases in disorder it necessarily loses heat.

$$\Delta G = \Delta H - T\Delta S \tag{16}$$

Table 2-2 – Conditions for reactions spontaneity

	$\Delta H<0$	$\Delta H>0$
$\Delta S<0$	*Spontaneous at low T* ($\lvert T\Delta S\rvert$ *is lower than* $\lvert \Delta H\rvert$)	*Non spontaneous at any T* $\Delta G>0$
$\Delta S>0$	*Spontaneous at all T* $\Delta G<0$	*Spontaneous at high T* ($T\Delta S$ *is greater than* ΔH)

---

[4] A thermodynamic quantity equivalent to the internal energy of the system plus the product of pressure and volume. Enthalpy includes the internal energy, which is the energy required to create a system, and the amount of energy required to make room for it by displacing its environment and establishing its volume and pressure (*Zemansky, 1968).*

Gibbs work took some time to become known by other scientists and the 1923 textbook "*Thermodynamics and the Free Energy of Chemical Substances"* by Gilbert N. Lewis and Merle Randall was essential in spreading that knowledge and finally replace the idea of affinity by the idea of free energy as the driving force in a chemical reaction. Nevertheless the affinity table is seen as a predecessor for Gibbs free energy since it was a first way of predicting the course of a reaction (Thims, 2007).

In modern terms chemical equilibrium can be defined as a minimum energy state. The idea of affinity was replaced by the idea of free energy as the driving force in a chemical reaction.

Summarizing, presently, from a kinetic point of view, chemical equilibrium is determined by a quantitative expression (still very similar to the one presented by Van't Hoff) as well as an interpretation of the phenomenon at microscopic level based on the collisions theory. We know that the occurrence of a certain reactions, in the gas phase, result from effective collisions between the particles, which lead to the formation of new substances. If, between these new substances exist features that allow for effective collision, the reverse reaction can also occur. The simultaneous occurrence of the reaction in both directions means that part of the reagent consumed in the forward reaction is produced by the reverse reaction. However, given the initially greater amount of reagents, the reaction occurs at a higher speed in the forward direction, this speed goes down as the concentration of product is increased, which on the other hand raises the speed of the reverse reaction (Figure 2.25). Thus, if the reaction system is closed, avoiding the loss of reagents or products, the reaction can progress to a state where there aren't any macroscopic changes in variables, the aforementioned equilibrium state. However, this state is far from static, as microscopically the forward and reverse reactions never cease to occur; they simply proceed with equivalent (speed. For this reason the Chemical Equilibrium is often called dynamic equilibrium.

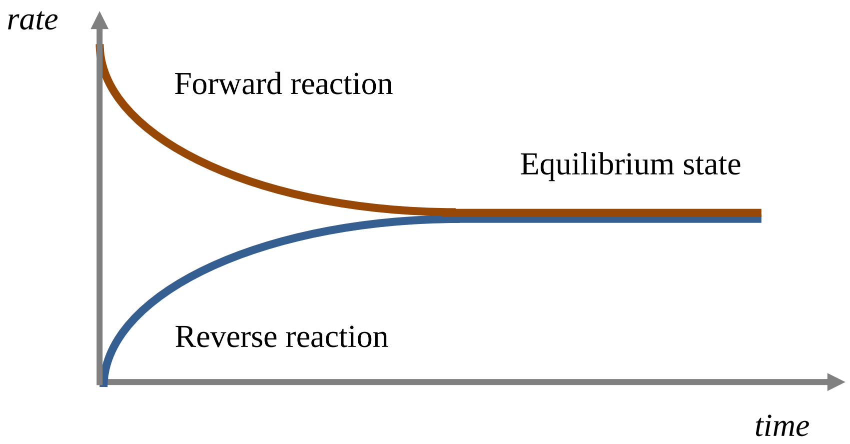


Figure 2-25 Evolution of reaction rates until chemical equilibrium state is reached.

Some authors prefer a thermodynamic approach while others opt for a kinetic approach. For a given reaction to occur significantly in both directions, it needs to be brought together both the thermodynamic and kinetic conditions. Energy determines the extent of reaction and the kinetics the timely occurrence of the same. Starting from either of these approaches, the quantification of the extent to which a chemical reaction occurs is based on the equilibrium constant. The larger the equilibrium constant, the greater the extent of the reaction in the direction for which it is calculated. The quantification of chemical equilibrium in terms of the amount of product formed compared to the amount of reagent provided is essential, for example, for the chemical of productivity in industry.

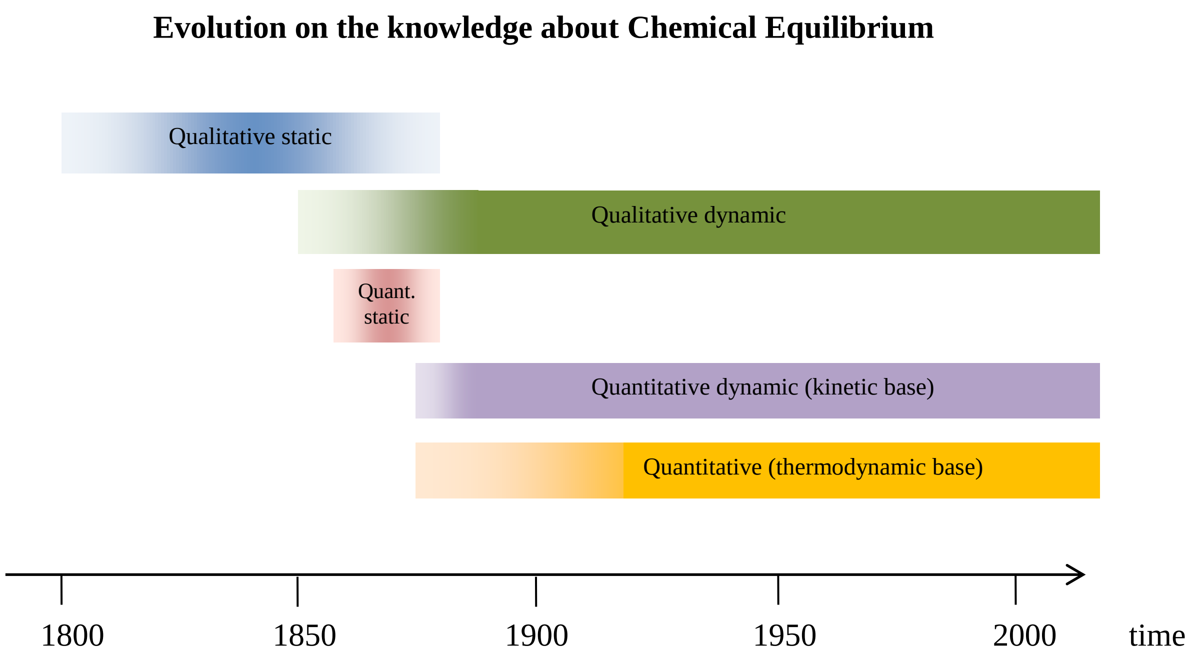
Banerjee (1995), for example, believes that thermodynamics is the most logical way to discuss the Chemical Equilibrium, since the equilibrium laws are based on thermodynamics. One of the major drawbacks associated with the kinetic approach relates to the application of mathematical expressions only to elementary reactions. To reach a broader equation for the Chemical Equilibrium, based on kinetic theories is necessary to use more complex explanations (Van Driel & Gräber, 2002). Nevertheless, at a basic level, kinetics can provide an answer while avoiding the need to understand thermodynamic expressions and variables. Nowadays, in advanced chemistry textbooks, Chemical Equilibrium usually combines mathematical treatment resulting from both kinetic and thermodynamic approaches and microscopic explanations in the domain of molecular kinetics. The usual sequence (Chang, 2005; Atkins, 1998; Brown et al., 2012) is to start by a chapter about chemical kinetics, usually presenting reactions as occurring in one direction only. In the next chapter are presented reversible reactions and chemical equilibrium. Thermodynamics is saved for a later chapter at which a new look is taken at the equilibrium constant from energetic considerations. This discussion will be exploited in Chapter 3, in which pedagogical concerns will be on the table.

According to Quílez, 2009, in the literature there is outlined the historical sequence: elective affinities (forces) → affinities/mass of reactants/static equilibrium → concentration of reactants/static equilibrium (forces) → dynamics/rates of forward and reverse reactions in equilibrium → thermodynamics. From the historical review made above, we present our own interpretation of the evolution in the concept of Chemical Equilibrium. We think Chemical Equilibrium concept evolved in two different fields:

1. from a static to a dynamic interpretation of the phenomenon;

2. from a qualitative to a quantitative knowledge of the phenomenon.

Also the changes in the understanding of the concept didn’t occur drastically but instead gradually. Initially, Chemical Equilibrium was approached qualitatively based on a static model. These ideas were then abandoned by a dynamic model of Chemical Equilibrium, still used nowadays to explain qualitatively the phenomenon. Nevertheless, although dynamic equilibrium emerged by the middle of the nineteenth century, the static perspective prevailed for some time, being the first to inspire a quantitative description of Chemical Equilibrium. So, the dynamic qualitative view of Chemical Equilibrium coexisted with the first attempts to quantify equilibrium based on a static view of the phenomenon. This context didn’t last long and mathematical expressions were quickly reformulated on the light of kinetics. Quantitative developments based on thermodynamics were contemporary to kinetic formulations. Despite this, the value of thermodynamic treatment was recognized much later. Both of them prevail “in equilibrium” nowadays. The chronologic bar presented on figure 2.26 contextualizes this evolution the concept of CE and summarizes the historical review made along this section.



Evolution on the knowledge about Chemical Equilibrium

Figure 2-26 Chemical equilibrium concept development.

Now, we try to locate the different “phases” of Chemical Equilibrium concept, according to the zones of chemistry knowledge space - the triangle proposed on section 2.1.

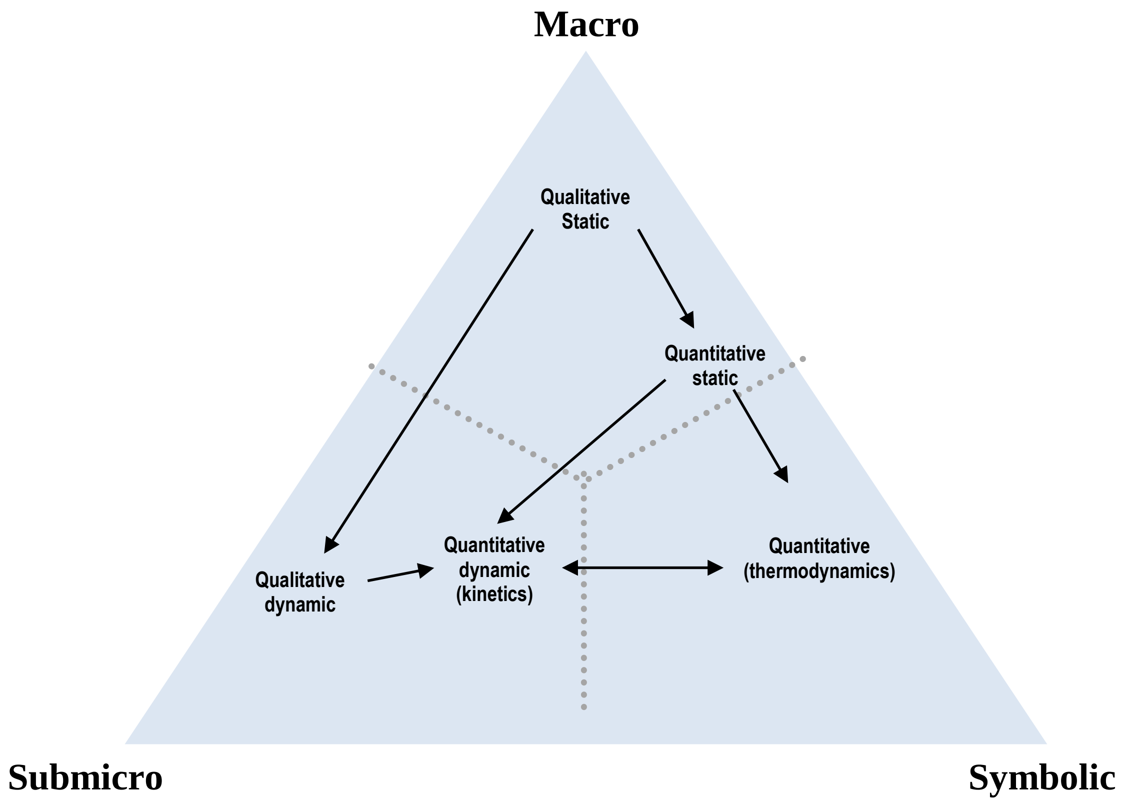


Figure 2-27 Chemical equilibrium concept development.

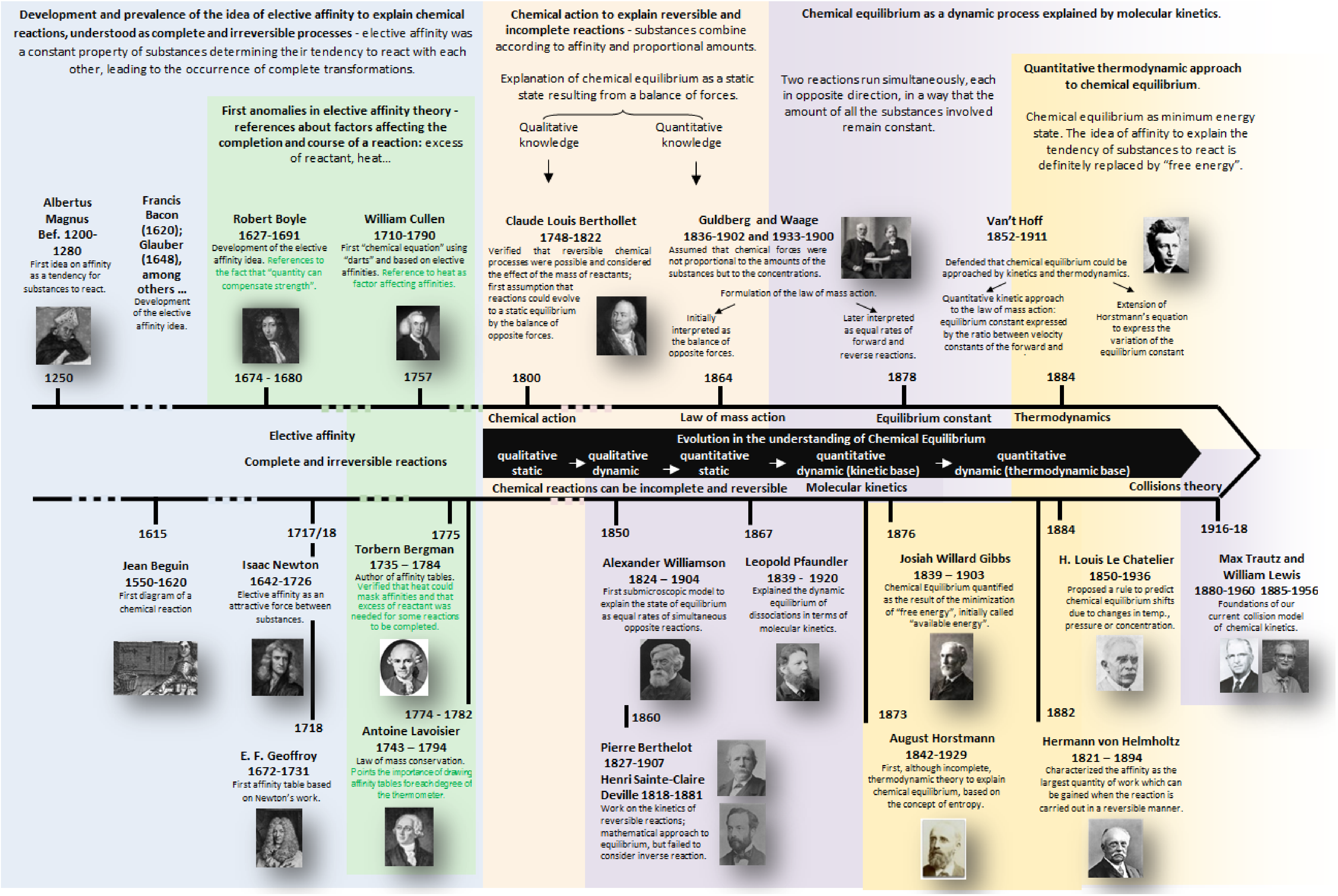
The first clues to Chemical Equilibrium were mainly based on observations and so the preliminary model was predominantly macro in character: chemical equilibrium was seen as a state at which reactants and products coexisted by a balance of opposite forces but the character and cause of this forces were unknown. From this point, the evolution took two different roads. For one side it evolved to a dynamic perspective, taking the discussion around equilibrium to the sub-micro level in order to understand the molecular events that lead to the equilibrium state. On the other hand the concept has also grown in symbolic character with the search for an expression to describe equilibrium state. At first, the quantification was based on empirical data and so macro dominant. Later, based on both the quantitative and qualitative reasonings, a dynamic quantitative treatment of chemical equilibrium on a kinetic base was achieved for simple reactions. This model was now more equilibrated in the three domains, starting to reflect the triple character of

Chemical Equilibrium: includes a model that explains the events at the submicro scale (collisions theory), the prediction and coherence with the consequences at macro scale and the quantification of the equilibrium state as well as symbolic representation of reactions according to reversibility and dynamism ideas.

Finally, thermodynamic prediction and quantification of the equilibrium state came to complete this scenario. Thermodynamics, developed in close interaction with kinetics (justifying the two-way arrow), allowed the application of mathematical expressions to more complex reactions "completing" the symbolic domain. Johnstone refers that thermodynamics operates on macro and symbolic levels only (Johnstone, 1982): "Any suggestion that a macro study is intellectually inferior can be refuted if one reflects upon the nature of classical thermodynamics which operated on descriptive and representational levels only". Although this is true for classical thermodynamics, in the case of Chemical Equilibrium we think that some micro character is present since energetic considerations ground on the events occurring at molecular level. When applying thermodynamics to chemical processes the meaning of concepts like enthalpy and entropy is based on considerations at the submicro domain, such as the energy of molecular bonds from reactants and products or the number of microstates. Nevertheless, it is also important to notice that this microscopic interpretation of entropy and enthalpy in a chemical reaction, that we have already referred when exposing the thermodynamic view of equilibrium, is very frequently left of, even at advanced chemistry approaches of Chemical Equilibrium. So, these roots are usually "accessory" at the level that thermodynamic knowledge is used in the context of Chemical Equilibrium, centring the purpose on the mathematical treatment and the reflections on the system at macro scale variables and quantities. As Johnstone concludes: "statistical thermodynamics uses all three levels and has given us new insights, but that in no way detracts from the power of the classical macro study". The arrow from quantitative static view to thermodynamics (figure 2.27) is justified from the interpretation that affinity tables were a first way of predicting the course of a reaction being an early predecessor of Gibbs free energy (Thims, 2007). Also, it is interesting to notice that Gibbs free energy is a construct that helps to more effectively analyze the course of a reaction but the true chemical and physical character resides in the concepts of enthalpy and entropy. Gibbs free energy detains a more symbolic nature, reason why several authors prefer to call it Gibbs function.

From this analysis we can conclude that the first theories about CE were mainly focused in the macro domain. Nevertheless, those did not last to the present, showing the importance of using the micro and symbolic characters in order to create a more satisfactory model to explain CE. Also, it is interesting to reflect on the fact that the most predictive treatment of equilibrium is the one that has the most symbolic character (thermodynamics). Even with this, the model based in kinetics is probably the most explanatory one. Finally, it is also important to note that although both qualitative and quantitative static views were replaced by other approaches, the content related to the observations and measurements of reactions at macro level prevail until our days as a macro component of Chemical Equilibrium.

To close this historical review we present a scheme illustrating the evolution in the knowledge about chemical reactions and the major personalities involved.



Development and prevalence of the idea of elective affinity to explain chemical reactions, understood as complete and irreversible processes - elective affinity was a constant property of substances determining their tendency to react with each other, leading to the occurrence of complete transformations.

First anomalies in elective affinity theory - references about factors affecting the completion and course of a reaction: excess of reactant, heat…

Chemical action to explain reversible and incomplete reactions - substances combine according to affinity and proportional amounts.

Explanation of chemical equilibrium as a static state resulting from a balance of forces.

Qualitative knowledge

Quantitative knowledge

Chemical equilibrium as a dynamic process explained by molecular kinetics.

Two reactions run simultaneously, each in opposite direction, in a way that the amount of all the substances involved remain constant.

Quantitative thermodynamic approach to chemical equilibrium.

Chemical equilibrium as minimum energy state. The idea of affinity to explain the tendency of substances to react is definitely replaced by "free energy".

Albertus Magnus
Bef. 1200-1280
First idea on affinity as a tendency for substances to react.
1250

Francis Bacon (1620); Glauber (1648), among others …
Development of the elective affinity idea.

Robert Boyle
1627-1691
Development of the elective affinity idea. References to the fact that "quantity can compensate strength".
1674 - 1680

William Cullen
1710-1790
First "chemical equation" using "darts" and based on elective affinities. Reference to heat as factor affecting affinities.
1757

Claude Louis Berthollet
1748-1822
Verified that reversible chemical processes were possible and considered the effect of the mass of reactants; first assumption that reactions could evolve to a static equilibrium by the balance of opposite forces.
1800

Guldberg and Waage
1836-1902 and 1933-1900
Assumed that chemical forces were not proportional to the amounts of the substances but to the concentrations.

Formulation of the law of mass action.

Initially interpreted as the balance of opposite forces.
1864

Later interpreted as equal rates of forward and reverse reactions.
1878

Van't Hoff
1852-1911
Defended that chemical equilibrium could be approached by kinetics and thermodynamics.

Quantitative kinetic approach to the law of mass action: equilibrium constant expressed by the ratio between velocity constants of the forward and

Extension of Horstmann's equation to express the variation of the equilibrium constant
1884

Chemical action | **Law of mass action** | **Equilibrium constant** | **Thermodynamics**

Elective affinity

Complete and irreversible reactions

Evolution in the understanding of Chemical Equilibrium

qualitative static → **qualitative dynamic** → **quantitative static** → **quantitative dynamic (kinetic base)** → **quantitative dynamic (thermodynamic base)**

Chemical reactions can be incomplete and reversible | **Molecular kinetics** | **Collisions theory**

1615
Jean Beguin
1550-1620
First diagram of a chemical reaction

1717/18
Isaac Newton
1642-1726
Elective affinity as an attractive force between substances.

1718
E. F. Geoffroy
1672-1731
First affinity table based on Newton's work.

1775
Torbern Bergman
1735 – 1784
Author of affinity tables. Verified that heat could mask affinities and that excess of reactant was needed for some reactions to be completed.

1774 - 1782
Antoine Lavoisier
1743 – 1794
Law of mass conservation. Points the importance of drawing affinity tables for each degree of the thermometer.

1850
Alexander Williamson
1824 – 1904
First submicroscopic model to explain the state of equilibrium as equal rates of simultaneous opposite reactions.

1860
Pierre Berthelot
1827-1907
Henri Sainte-Claire Deville 1818-1881
Work on the kinetics of reversible reactions; mathematical approach to equilibrium, but failed to consider inverse reaction.

1867
Leopold Pfaundler
1839 - 1920
Explained the dynamic equilibrium of dissociations in terms of molecular kinetics.

1876
Josiah Willard Gibbs
1839 – 1903
Chemical Equilibrium quantified as the result of the minimization of "free energy", initially called "available energy".

1873
August Horstmann
1842-1929
First, although incomplete, thermodynamic theory to explain chemical equilibrium, based on the concept of entropy.

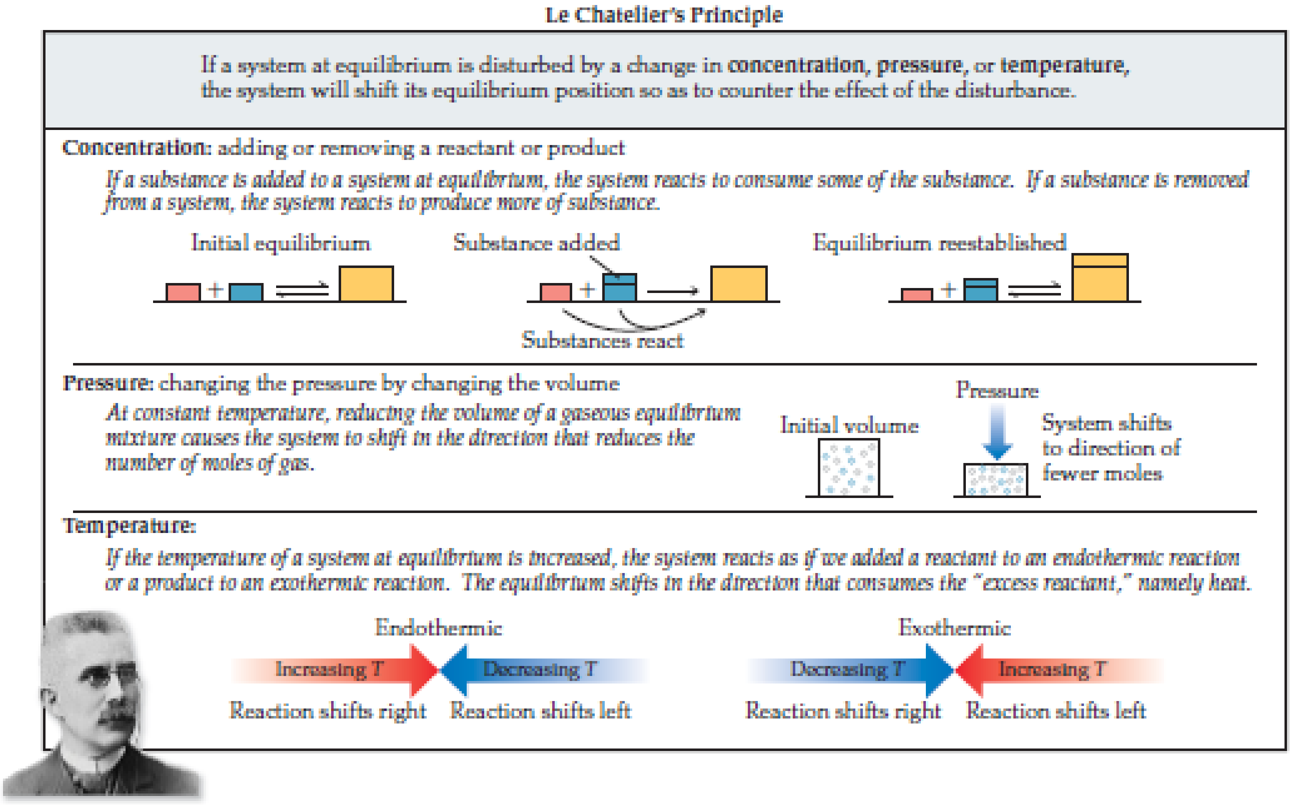
1884
H. Louis Le Chatelier
1850-1936
Proposed a rule to predict chemical equilibrium shifts due to changes in temp., pressure or concentration.

1882
Hermann von Helmholtz
1821 – 1894
Characterized the affinity as the largest quantity of work which can be gained when the reaction is carried out in a reversible manner.

1916-18
Max Trautz and William Lewis
1880-1960 1885-1956
Foundations of our current collision model of chemical kinetics.

Chemical equilibrium involves not only the attainment of the dynamic state already described, but also the understanding of the factors affecting the equilibrium state, the consequences of the disturbances and the conditions for reestablishing equilibrium. So, in a concept that is by itself dynamic we have to include the added complexity of changing conditions and predict the effect of those changes, a process essential to the use of this concept in real life events.

Le Chatelier, in 1884, adapted Van't Hoff's mobile equilibrium principle proposing a simple rule aimed to predict chemical equilibrium shifts due to changes in temperature, pressure or concentration. Nowadays, this rule has been restated by several chemistry textbooks, becoming very popular among chemistry educators. Figure 2.28 is presented as an example of the use of Le Chatelier's principal in a text book.


Le Chatelier's Principle

If a system at equilibrium is disturbed by a change in **concentration, pressure,** or **temperature,** the system will shift its equilibrium position so as to counter the effect of the disturbance.

Concentration: adding or removing a reactant or product

If a substance is added to a system at equilibrium, the system reacts to consume some of the substance. If a substance is removed from a system, the system reacts to produce more of substance.

Pressure: changing the pressure by changing the volume

At constant temperature, reducing the volume of a gaseous equilibrium mixture causes the system to shift in the direction that reduces the number of moles of gas.

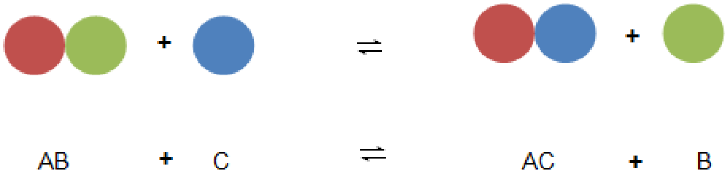
Temperature:

If the temperature of a system at equilibrium is increased, the system reacts as if we added a reactant to an endothermic reaction or a product to an exothermic reaction. The equilibrium shifts in the direction that consumes the "excess reactant," namely heat.

Figure 2-28 Le Chatelier principle (Brown et al, 2012).

Chemical equilibrium disturbances can be analyzed according with a kinetic and a thermodynamic base instead of using Le Chatelier's principle which is a type of algorithm.

To help visualize the effects of disturbances to equilibrium we will use the notation from figure 2.24 and the reaction from figure 2.21, supposing that al the species are in gaseous state:



The addition or removal of species involved in the reaction is the most common process when we refer to the disturbance of equilibrium state by changes of concentration.

According to the Le Chatelier's principle, one can predict that the addition of a reagent to a system in equilibrium will cause it to move in order to counteract the increase in concentration imposed, which will only be achieved with the displacement of the Equilibrium in the forward direction (reagent consumption and product formation). However, this prediction by the Le Chatelier's principle is only valid if the addition of reagent is carried out at constant volume and temperature conditions.

When a reagent is added, while at constant volume and temperature, the concentration of this reagent increases. However, the concentrations of the remaining constituents stay the same, since none of the factors that determine them vary. Following we present the expression of equilibrium constant for this reaction:

$$K = \frac{|AC|_{eq}|B|_{eq}}{|AB|_{eq}|C|_{eq}} \tag{17}$$

When the system isn't at equilibrium state, we can write reaction quotient:

$$Q = \frac{|AC||B|}{|AB||C|} \tag{18}$$

So, using this expression, we can verify that the increase in the concentration of one of the reactants leads to $Q < K$ and therefore the system will have to evolve towards the formation of products, where Q increases to equalize with K. This displacement towards the formation of products is one of the reasons why, in several industrial applications an excess of reagent is added to the established equilibrium.

Using a kinetic interpretation, based on the collisions theory, we concluded that the greater number of reagent particles, present due to the addition, leads to the existence of a greater number of collisions between the particles of the reactants. This, results in a momentary increase in the rate of direct reaction (Tyson et al., 1999), which then decreases as the rate of the reverse reaction increases, until a new equilibrium state is established. Thus, there is an increase in the concentration of the products in the new equilibrium the rate of the direct and inverse reactions are both higher than in the previous equilibrium.

Figure 2.29 shows the effect of adding reactant to a system in equilibrium for the hypothetical reaction that is accompanying us along the chapter. Suppose that the first image (I) shows an equilibrium state. Consider adding some amount of reactant C to the equilibrium (II). In figure III we can see the new equilibrium established.

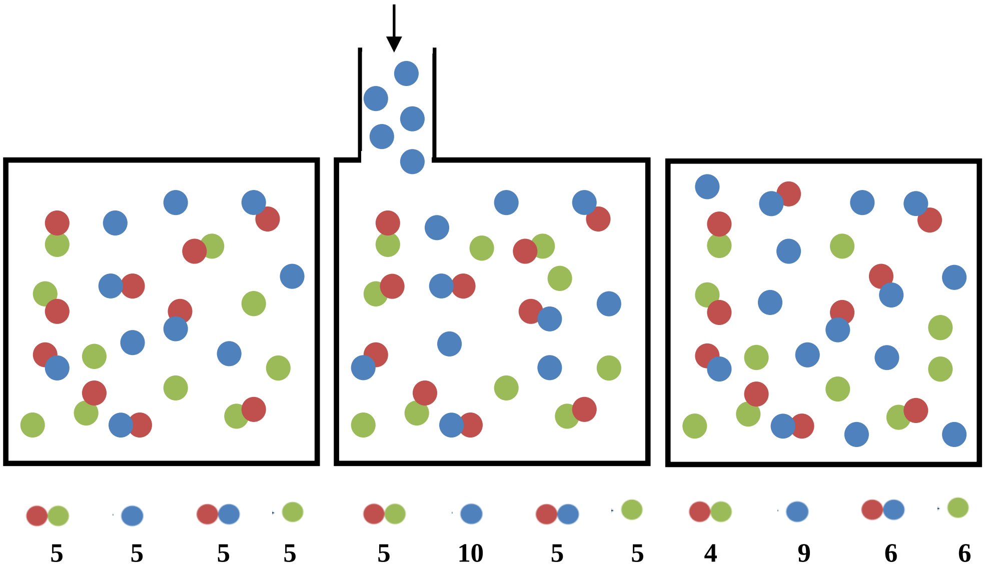


Figure 2-29 Equilibrium disturbance and reestablishment by addition of a reactant.

Some of the added reactant is spent, but note that at the new equilibrium the constant must be the same, so the ratio is similar as “simulated” for the particles represented in the figure.

$$\frac{(5\times5)}{(5\times5)}=\frac{(4\times9)}{(6\times6)} \tag{19}$$

It should also be noted that the amount of reactant C in the second equilibrium, although decreased with respect to the quantity at the time of addition, is in any case greater than that existing in the first equilibrium.

Addition of a reaction product or withdrawal of a reagent, at constant temperature and volume, will obviously have an effect contrary to that noted above.

These results correspond, as already mentioned, to the addition of reagents at constant volume and temperature. This is the most common case studied during the teaching of Chemical Equilibrium. Working in open systems, where pressure is maintained, while volume is variable, the equilibrium response to the disturbance is different (Solaz & Quílez, 2001) as treated in our own previous work (Fonseca, 2006).

Another factor affecting equilibrium state is the variation of the total pressure, which influences, in particular, systems with gaseous constituents. In the first place, it is necessary to distinguish between two forms of varying total pressure of a reactional system: by an injection of an inert gas, which has also been thoroughly investigated during previous work on a master's degree (Paiva et al., 2008) or by decreasing the volume. Suppose that the total pressure of the system for the ammonia synthesis is increased by decreasing the volume, at constant temperature. Writing the reaction equation,

$$N_2\,(g) + 3H_2\,(g) \rightleftharpoons 2NH_3\,(g) \tag{20}$$

According to Le Chatelier's principle, the system's response will be to reduce the pressure. For this, the equilibrium will tend to move towards the formation of the smallest number of moles of gaseous species. There are four moles of gaseous species in the reactants and two moles of gaseous species in the products, whereby the equilibrium will move in the direct direction, favoring the formation of ammonia. In systems whose number of moles of gaseous species is similar in reagents and in products, there is no influence on the part of the variation of the total pressure by volume change. That is what happens with the example reaction we are using along the chapter and represented in figure 2.30.

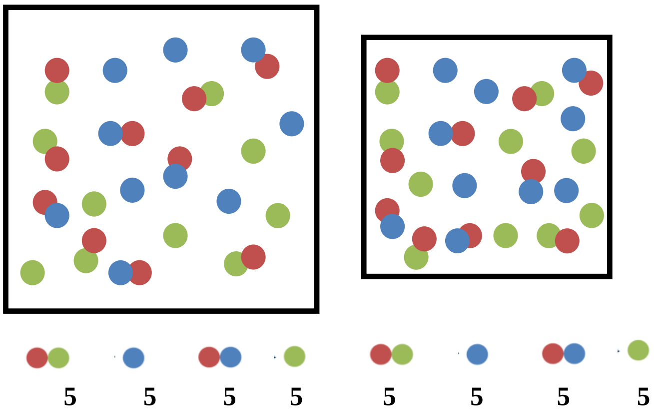


Figure 2-30 Equilibrium disturbance by volume change in a system in which the number of moles of gaseous species is similar in reagents and in products,

In order to analyze the situation from a quantitative point of view, it is necessary to use other resources in addition to the Le Chatelier's principle. From the thermodynamic point of view it is verified that the equilibrium constant depends on the value of $\Delta_r G^o$, which is defined at the standard pressure. Thus, $\Delta_r G^o$ and therefore K, do not depend on the total pressure of the system at which equilibrium is established (Atkins, 1998). However, although the K value does not vary with the pressure, the equilibrium composition is not necessarily pressure independent. Consider the equilibrium constant in terms of pressures[5] for the ammonia synthesis,

$$K_p = \frac{p^2_{(NH_3)\,eq}}{p_{(N_2)\,eq}\; p^3_{(H_2)\,eq}} \tag{21}$$

in which the quantities represented correspond to equilibrium pressures, for a given composition of the system. Any change in total pressure that influences the equilibrium state should imply the variation of the partial pressure of the species involved in the reaction, so that the ratio between them in equation 21 changes. In this case, since the

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[5] From the perfect gases law:

$$PV = nRT$$

which relates the variables P (pressure), T (temperature), n (amount of substance) and V (volume), while R represents the perfect gases constant, it is possible to establish the relation between K_c and K_p:

$$Kp = Kc\,(RT)^{\Delta\nu}$$

Where $\Delta\nu$ is equal to the difference between the sums of the stoichiometric coefficients of the gaseous products and the stoichiometric coefficients of the gaseous reactants.

partial pressures are no longer those of equilibrium, the above equation corresponds to the quotient of the reaction:

$$Q_p = \frac{p^2_{(\mathrm{NH_3})}}{p_{(\mathrm{N_2})}\, p^3_{(\mathrm{H_2})}} \tag{22}$$

But how does the variation in total pressure affect the change in partial pressures? To answer this question, we need to remember the perfect gas law by writing it, in the case of a component A from a reactional mixture

$$p_\mathrm{A} = \frac{n_\mathrm{A} RT}{V} \tag{23}$$

with $\underline{n}_\mathrm{A}$ being the amount of substance of component A in the mixture, R the perfect gases constant, T the temperature and V the volume of the system.

Assuming that p_A is the pressure of reactant A at the equilibrium, by doubling the total pressure (in the instant $t_{1)}$, at constant temperature, the volume is reduced by half, then:

$$p_\mathrm{A}(t_1) = \frac{n_\mathrm{A} RT}{\frac{1}{2}V} = \frac{2n_\mathrm{A} RT}{V} \tag{24}$$

Given that p_A (t_1) = $2p_A$, one can write the reaction quotient, as

$$Q_p = \frac{2^2\, p^2_{(\mathrm{NH_3})\,\mathrm{eq}}}{2p_{(\mathrm{N_2})\,\mathrm{eq}}\; 2^3\, p^3_{(\mathrm{H_2})\,\mathrm{eq}}} = \frac{1}{4}\cdot\frac{p^2_{(\mathrm{NH_3})\,\mathrm{eq}}}{p_{(\mathrm{N_2})\,\mathrm{eq}}\; p^3_{(\mathrm{H_2})\,\mathrm{eq}}} \tag{25}$$

Since $Q_p < K_p$, the equilibrium will move in the forward direction (formation of reaction products) in order to increase the value of Q_p until it returns to the value of K_p. The analysis in terms of the equilibrium constant is, therefore, according to the Le Chatelier´s principle.

It is important to note that when the total pressure is increased, the partial pressure of all the substances present will increase. Although the equilibrium moves towards the smaller number of moles of gaseous species, all partial pressures will be higher at the new equilibrium than the initial equilibrium. Only the molar fraction of the species consumed in the equilibrium displacement decreases (Knox, 1985). In the same way, decreasing the pressure of the system, regardless of the fact that it causes its displacement towards the production of the largest number of moles of gaseous species, represents the decrease of all partial pressures in the new equilibrium (Allsop & George, 1984).

The conclusion that pressure variations do not affect reactions with $\Delta\nu = 0$ is easily obtained with the analysis in terms of equilibrium constant previously performed, since cancelation of the stoichiometric coefficients occurs, maintaining the ratio between the partial pressures.

From the kinetic point of view, changes in equilibrium can be interpreted on the basis of collisions theory. In pressure's case, a rise of this variable will increase the concentration of the species present in the system, due to the decrease of the volume. This, in turn, will increase the rate of the forward and reverse reactions. However, the increase will be more noticeable in the presence of more moles of gaseous species (due to the increase of the concentrations to the respective stoichiometric coefficients), so that the reaction will evolve towards the consumption of these species until a new equality is verified between the rates of the two reactions.

Changes in either the quantities of reagents or products and changes in pressure lead to a restoration of equilibrium trough a return to the value of K. This happens because these changes do not directly interfere with the value of K, since they do not influence $\Delta_r G^o$, which determines it. Thus, the partial pressures (and consequently concentrations) are adjusted until G reaches a minimum (David, 1988).The temperature, being another of the factors that influence the balance, has a particular character.

The Le Chatelier principle predicts that the equilibrium of a reaction system will tend to shift in the endothermic direction if the temperature increases, since there will be absorption of thermal energy counteracting the effect of temperature rise. Conversely, the equilibrium will shift in the exothermic sense if the temperature decreases, opposing the disturbance by heat release (Atkins, 1998).

The shift direction of Chemical Equilibrium with temperature variations is therefore dependent on the reaction being exothermic or endothermic. In an exothermic reaction the enthalpy change is negative, i.e., heat is released. On the other hand in an endothermic reaction, the enthalpy is positive, corresponding to the consumption of heat by the system, at constant pressure and temperature.

For the synthesis of ammonia, the direct reaction is found to be exothermic, $\Delta_r H$ = - 92 kJ mol^{-1}. The energy released in the formation of the products is higher than that consumed in the breakdown of the reagent bonds. Since the direct reaction is exothermic, the reaction in the reverse direction will be endothermic. Thus, by raising the temperature, the equilibrium moves in the opposite direction, that is, in the sense of ammonia consumption and reagent formation. It is concluded that with respect to temperature, the formation of ammonia will be favored by lower temperatures. From the thermodynamic point of view, it is found that the temperature acts directly on the reaction equilibrium constant, changing its value. This is because this factor influences the tendency for reaction to occur.

The influence of temperature on Chemical Equilibrium can be analyzed by equating equations 13 and 16:

$$\Delta_r H^o - T\Delta_r S^o = - RT \ln K \tag{25}$$

Solving in order to K:

$$\ln K = \frac{\Delta_r S^o}{R} - \frac{\Delta_r H^o}{RT} \tag{26}$$

The effect of T in K is related to the term $\Delta_r H^o$, namely with its signal (Reger et al., 1997). Thus, since the variation in K implies alteration of the equilibrium, the signal of ΔH^o is the determinant of the direction of displacement with temperature. Van't Hoff called this principle the mobile equilibrium (Treptow, 1980). Thus, if ΔH^o is negative, the increase in temperature will decrease the equilibrium constant favoring the production of reagents, with the opposite occurring if ΔH^o is positive.

Regarding kinetics, the effect of temperature under Chemical Equilibrium is interpreted while taking into account that reactions with higher activation energies are more influenced by temperature. In an exothermic reaction, the reverse reaction has higher activation energy than direct reaction, so with an increase in temperature, the rate of the reverse reaction will increase more than the rate of the direct reaction (Reger et al., 1997).

The ratio between specific rates and consequently the equilibrium constant is thus changed. It should be noted that although one reaction is more favored than another, the speed of both increases with a rise in temperature.

For the system shown in Figure 2.31, where the reaction is exothermic, the increase in temperature will correspond to the displacement towards the formation of reagents. Note that now, unlike previous cases, the fraction between product and reagent particles should vary, indicating change in the equilibrium constant itself. The variation from

$$\frac{(5 \times 5)}{(5 \times 5)} \text{ to } \frac{(4 \times 4)}{(6 \times 6)}$$

was chosen as an example.

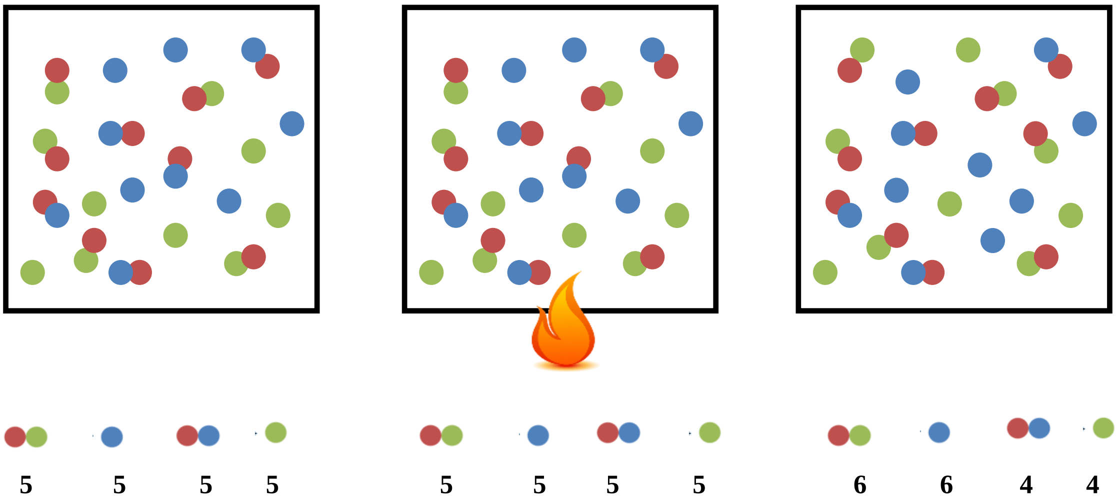


Figure 2-31 Equilibrium disturbance by temperature change in an exothermic reaction.

Table 2.3 summarizes the reasoning involved in the understanding of some typical disturbances made to systems in equilibrium state according to different approaches.

Table 2-3 Equilibrium displacement and reestablishment

Disturbance **Approach**	**Concentration** ***Adding reactant at constant V and T***	**Pressure** ***Rising the total pressure by diminishing the volume of the system, at constant T***	**Temperature** ***Rising the Temperature of an Exothermic reaction***
Le Chatelier's principle	The system will shift equilibrium's position so as to counteract the effect of the disturbance: displacement in the forward direction to consume reactants.	The system will shift equilibrium position so as to counteract the effect of the disturbance: displacement in the direction with a lesser number of gaseous moles (in order to diminish pressure).	The system will shift equilibrium's position so as to counteract the effect of the disturbance: displacement in the direction that decreases temperature (absorbs energy), inverse reaction for an exothermic process.
Kinetics	A growth in the concentration of one of the substances participating in the reaction will cause a rise in the number of effective collisions and favor the reaction in which that substance is transformed, in this case, forward direction.	A growth in the total pressure will increase the partial pressures from all substances participating in the reaction, which leads to an increase of the forward and reverse reaction rates. Nevertheless, the increase will be larger for a greater number of gaseous moles (more collisions) favoring the reaction in which those "extra" moles are consumed.	A growth in the temperature of the system will raise the number of effective collisions. In this way, the reaction with higher activation energy will be more favored. In the case of an exothermic process the inverse reaction has got higher activation energy.
Quantitative /Thermo-dynamical	*K* value does not change since $\Delta_r G^o$ remains constant. Nevertheless, a growth in the concentration of one of the reactants leads to $Q < K$, shifting the equilibrium in the forward direction in order to get back to *K's* value, which means minimizing Gibbs free energy: $\Delta_r G = 0$	*K* value does not change since $\Delta_r G^o$ remains constant (since it is defined at standard pressure). Nevertheless, the variation in volume will change the partial pressures of the species involved in a reaction at gaseous phase. According to the stoichiometric coefficients it can occur that: $Q < K$; $Q > K$ or $Q = K$ which determines the shift of the equilibrium.	*K* value changes since *T* affects $\Delta_r G^o$. If ΔH^o is negative, the increase in temperature will decrease the equilibrium constant favoring the production of reagents (inverse reaction).

As referred in the beginning, Chemical Equilibrium is a theme simultaneously dependent and integrant of several concepts in chemistry. Chemical equilibrium problems involve not only the concepts that are unique to it, but also other concepts such as the mole and reaction stoichiometry, gases and the ideal gas law (Kousathana & Tsaparlis, 2002). We have reflected about the essential previous concepts involved in Chemical Equilibrium and elaborated table 2.4, decomposing the concepts in their major macro, micro and symbolic components.

Table 2-4 Prerequisite concepts for the understanding of Chemical Equilibrium decomposed in their major macro, micro and symbolic aspects.

Dominant Level	**Prerequisite concepts for CE**					
	Chemical elements, substances and structure of matter	**Mass, amount of substance and concentration**	**Chemical reaction**	**Properties of gases and related variables**	**Chemical Kinetics**	**Thermodynamics**
Macro	Perception of the variety of substances in nature Chemical Elements Evidences of particle theory of matter.	Idea of mass as quantity of matter. Molar mass Idea of concentration as the abundance of a component per volume. (ex: two tea spoons of sugar in a water bottle).	Perception of the phenomenon of chemical change in nature. Conceptualization of chemical reactions as transformation into different substances. Quantitative empirical data from reactions. Verification of the law of mass conservation.	Pressure - force per area; Volume - space occupied; Temperature - intuitive idea of hot and cold. Properties of gases: behaviour at macroscopic level - occupation of available volume; compressibility…	Intuitive idea of reaction rate (comparing faster/slower reactions with daily life examples) Reaction rate experimental measurement	Classical thermodynamics energy, entropy and enthalpy concepts Heat Work
Micro	Atoms, ions and Molecules Electronic configuration and reactivity Elementary /composed and molecular/ionic substances. Molecular models according to Dalton's model of the atom.	Atomic/Molecular mass. Avogadro's number	Chemical reactions as a process of rearrangement of atoms. Chemical reactions as a process of electronic sharing and exchange. Law of mass conservation at atomic level Reaction stoichiometry	Kinetic-molecular theory of gases: properties of gases explained at molecular level.	Collisions theory on the explanation of factors affecting rate of reaction. Reaction mechanism	Statistical mechanics entropy concept - based on the number of possible microscopic configurations Enthalpy of reaction – in terms of bond energies
Symbolic / mathematical	Periodic Table Chemical symbols. Chemical formulas. Lewis structure	Mole concept – understood as a value/unity created to allow the use of reasonable quantities when dealing with substance amounts. Mole and Molarity calculations	Balanced chemical equations Calculations according to law of mass conservation	Perfect gases law	Rate law of a reaction Expressing the rate of a reaction as a time function	Thermodynamic mathematical relations between variables

Now, we focus on the new knowledge involved directly in the concept of Chemical Equilibrium. First, we state that Chemical Equilibrium thematic is mainly connected to the following ideas

- Reversible reactions
- Equilibrium state
- Equilibrium displacement and reestablishment

Table 2-5 Macro, micro and symbolic character in the ideas concerning Chemical Equilibrium.

Levels	Chemical Equilibrium base ideas		
	Reversible Reactions	**Equilibrium state**	**Equilibrium displacement and reestablishment**
Macro	Reversibility as the possibility of reactants and products to change roles - reaction may occur in both directions. Coexistence of reactants and products (incomplete reaction)	Equilibrium conceptualized as a static state where quantities remain constant Composition of a system in equilibrium Equilibrium state as a maximization of Universe entropy Equilibrium as a minimum energy state	Le Chatelier's principle experimental verification
Micro	Reversibility as the result of opposite reactions occurring simultaneously.	Dynamic equilibrium understood in terms of opposite simultaneous reactions occurring microscopically at the same rate. Chemical equilibrium establishment based on collisions theory. Equilibrium explained trough the balance in bond enthalpies and probabilities of Stefan Boltzmann's distribution (number of possible microstates);	Collisions theory applied to the disturbance and reestablishment of chemical equilibrium Le Chatelier's principle explanation
Symbolic / mathematical	Double arrow in chemical equations	Equilibrium law. Equilibrium condition based on Gibbs free energy.	Comparing equilibrium constant (K) and reaction quotient (Q) Le Chatelier's principle application Quantifying temperature dependence of equilibrium constant (K) thermodynamically.

Other kinds of categorization would certainly be possible, like the one referred by Quílez stating that three key basic ideas are recognized in the concept of Chemical Equilibrium: incomplete reaction, reversibility and dynamics (Quílez, 2004). Nevertheless, our choice reflects a connection to the traditional sequence used when approaching Chemical Equilibrium in education. In table 2.4 we analyze the presence of dominant macro, micro and symbolic character in the ideas concerning Chemical Equilibrium.

Rescuing our triangle of macro micro and symbolic domain from section 2.1, we organize the ideas from tables 2.4 and 2.5 (figure 2.32). This exercise in idea organizing will be useful in next chapter since it will be easier to analyze the macro micro or symbolic character of the common difficulties found in Chemical Equilibrium which, in turn, can help us understand how to minimize those difficulties. This will be the focus in the next chapter.

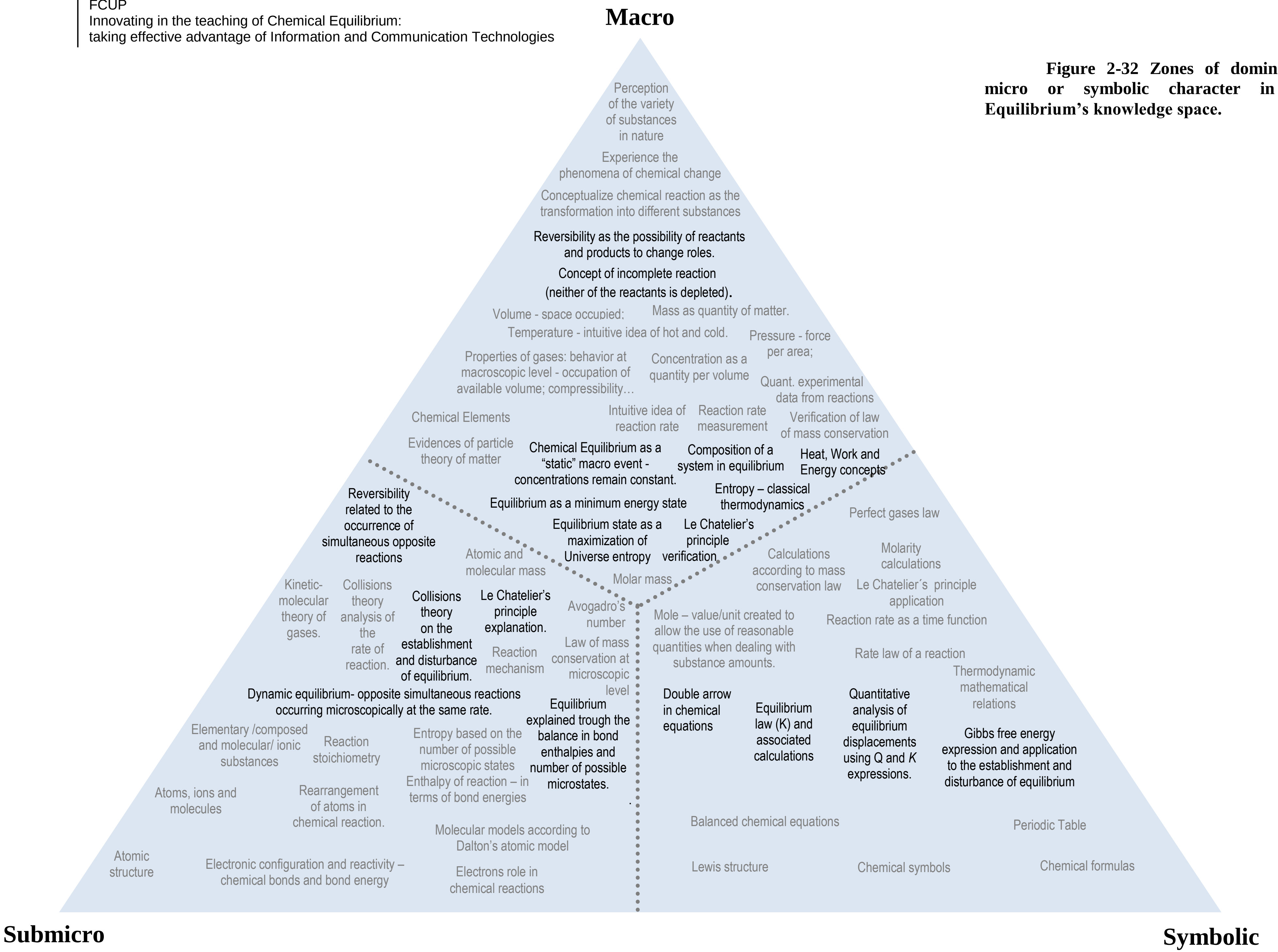


Figure 2-32 Zones of dominant macro, micro or symbolic character in Chemical Equilibrium's knowledge space.

Chapter 3 - Pedagogic dimension: Teaching Chemical Equilibrium

3.1. The understanding of formal concepts in chemistry

The review made along Chapter 2, provided good help with structuring ideas on the specific nature of chemistry. The result from that analysis can support us on identifying the major processes and difficulties present in the understanding of typical concepts in chemistry education.

In the literature there are several references pointing to the fact that chemistry operates at different levels as a determinant factor in the understanding of this science as well as the basis for several difficulties in its teaching. Stull *et al.* (2012) argues that for students to be successful in scientific disciplines, they must develop the skills of constructing, interpreting, and translating between various representations. This opinion is in accordance with the perspective that the understanding of chemistry involves interplay among macro, micro and symbolic levels, as presented already in Chapter 2. References usually point the need to integrate the knowledge from the micro and macro levels in order to meaningfully learn chemistry: “Understanding chemistry means knowing about properties of substances and how these relate to chemical structure and chemical bonding: these aspects are not separable.” (Barke & Wirbs, 2002). Talanquer (2011) also claims that each of the components of the triplet can be approached qualitatively or quantitatively, conceptually or algorithmically, depending on the nature of the task and the particular characteristics of both the teacher and the learner.

So, we can consider as one of the major features of learning chemistry the need to operate at different levels, constructing, interpreting and relating, knowledge from micro, macro and symbolic domains. However, it would be a mistake to imagine that all, or many, of our students can follow us up the middle of the triangle (Johnstone, 1991; Tsaparlis, 2001). In a study about chemical bonding, Halim *et al.* (2013) concluded that students have difficulties in seeing the shift or the connection between those particular levels and tend to build non-scientific mental models. So, they conclude it is important to help students visualize the concepts at the three levels and develop their scientific mental model. The same study also revealed that students have difficulties applying knowledge from the micro level to explain macro events: “Collected data shows that even though most of the students had the classical knowledge that all matter is made of particles; they failed to associate this scientific idea with daily-life events and to use it for explaining observed phenomena."

Devetak *et al.* (2009) created a model to explain the connection between the levels and points that the integrated mental model is a factor inducting knowledge into long term-memory (Figure 3.1).

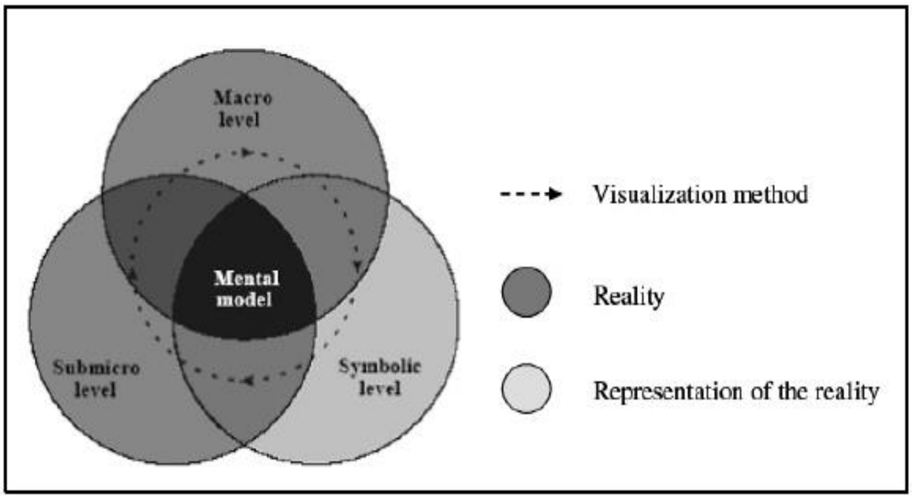


Figure 3-1 The interdependence of the three levels of science concepts model (after Devetak et al, 2009).

Yakmaci-Guzel and Adadan (2013) refer that in order to address the challenges students encounter while moving between all three levels of representation, researchers suggested engaging students with dynamic, multi representational visualizations of invisible phenomena, and among these are technologies that include animations and simulations of phenomena with multiple levels of representation.

Beside the fact that having to move between several levels is noticed as a challenge in itself (Potgieter et al., 2008), there are some levels considered to provide more difficulties than others. In the literature the difficulties related to the symbolic level in chemistry are frequently referred. Gabel (1999) states that the primary barrier to understanding chemistry, however, is not the existence of the three levels of representing matter. It is that chemistry instruction occurs predominantly on the most abstract level, the symbolic level (an idea previously reported by Johnstone). This level is the hardest one for students to understand, especially without understanding of the submicroscopic level of chemical concepts (Devetak et al., 2009). Potgieter *et al.* (2008) concluded that chemistry students find topics with a strong mathematical basis difficult to master. Hughes-Hallett (2001) cited by Potgieter *et al.* (2008) notes that mathematics focuses on climbing the ladder of abstraction and wants students to rise above context. Yet students have difficulty applying the mathematics they have learned in a different context. Although the fact that different subjects are taught separate from one another is part of the reason, recognizing mathematics in another field requires thorough understanding of the context. Nakhleh and Mitchell (1993) identified a reliance of students on algorithms to solve problems, even problems specifically intended for conceptual solution. The same tendency has been also diagnosed in more recent studies (Erdemir et al., 2000; Kousathana & Tsaparlis, 2002). Generally, students solve problems successfully using memorized algorithms. Many students who may be successful at solving mathematical problems do not understand the chemical concepts behind their memorized algorithmic solutions (Erdemir et al., 2000). Conceptual understanding may not be a prerequisite for applying algorithms, but it is very likely that if such understanding does exist, students are more capable of dealing with more demanding problems that require them to have overcome misconceptions and alternative conceptions (Kousathana & Tsaparlis, 2002).

The possibility of approaching the symbolic level from a micro or macro perspective can also complicate the understanding of chemistry: “To complicate matters more, chemists can represent both the macroscopic and the microscopic levels symbolically through the use of chemical symbols, chemical formulas, and chemical equations. The symbols that chemists use can be interpreted in several ways, like the symbol “Fe”, which can stand for one atom of iron or for a sheet of iron. “Because the three levels can be interpreted in more than one way, and because teachers unwittingly move from one level to another in lecturing, students fail to integrate the levels, which leads to a fragmented view of chemistry with many puzzling parts that do not seem to fit together. Helping students relate the three levels of representing matter has potential for improving conceptual understanding. An opportunity for doing this is through work in the laboratory” (Gabel, 1999).

Microscopic level is also commonly referred simultaneously as an important domain for the understanding of chemistry but also a factor of difficulty. Several studies have shown that students find microscopic and symbolic representations especially difficult because these representations are invisible and abstract while students' thinking relies heavily on sensory information. In addition, without substantial conceptual knowledge and visual-spatial ability, students are unable to translate one given representation into another. Gabel (1999) refers the importance of the microscopic level to fully understand properties at a macro level. What is observed and can be studied on the macroscopic level, can also be described on the microscopic level, and sometimes in so doing, the explanation appears to be more definitive. Submicro representations (SMR) could be an important element, not only for explaining the experimental observations to students, but also in the process of evaluating students’ knowledge and identifying their chemical misconceptions (Devetak et al., 2009).

Thus, the ability to make representations is held as an important operation to understand chemistry. If we think of the triangle of Figure 2.9 and the domains that it uncovers in chemical science, we easily recognize the weight of this process in its learning. On the one hand, representations constitute a way of communicating; a language specific to chemistry, so knowing how to use and interpret them is an essential process in understanding this science. However, the representations are more than this. The creation of symbolic representations is a way for chemists to structure their rationale both macroscopically and microscopically and to link these two domains: “As the discipline has developed, chemists have created different representations to develop a comprehensive understanding of chemical concepts, for example, molecular structure and reactivity” (Stull et al., 2012). Students construct representations based on partial understanding and then use the representations to improve their understanding (Potgieter et al., 2008). Chemistry concepts depend much on chemical representation and this contributes to the development of mental models (Halim et al., 2013). Thus, the chemical representations to which we are accustomed are the final result of a mental process of visualization of the scientific models. The concept of “representation” was described (many years ago) by Peirce (1955), stating that for a notation to function as a representation, someone has to interpret it and give it meaning, there by including three notions: something that is represented, the referring expression, and the interpretation linking the referring expression to that which is represented (Potgieter et al., 2008). According to this definition, tables, equations, and graphs become representations when someone gives them meaning by interpreting them. It is also noted that novice students have much less ability to construct or use scientific representations then science experts (Potgieter et al., 2008).

Gilbert (2005) points that “students of chemistry must have a mental model, of some kind, of an ‘atom’, all those of physics a mental model of a ‘force’, all those of biology a mental model of a ‘gene’, all those of earth science a mental model of a ‘tectonic plate’. By its very nature, a mental model is inaccessible to others. However, in order to facilitate communication, a version of that model must be placed in the public domain and can therefore be called an expressed model”.

Helping students to visualize models, building their own representations, is pointed as an important feature for them to better understand chemistry. One of the suggestions made in order to help students in this process of representing is the use of (external) models, which can aid in this process by allowing difficult internal processes to be replaced or augmented by external actions on models (Stull et al., 2012). Using physical objects to enact and support cognitively difficult tasks can enhance problem solving but it is safeguarded that the general lack of model use by some low performing participants suggests that a model-use strategy is not necessarily readily discovered or understood as relevant (Stull et al., 2012). The reference to the use of models is also commonly linked to the fact that chemistry involves many abstract and complex concepts (Halim et al., 2013). Gabel (1999) refers that many of the concepts studied in chemistry are abstract, and are “inexplicable without the use of analogies or models”.

Authors also refer that chemistry has been regarded as an especially difficult subject for young students by teachers, researchers and educators (Halim et al., 2013), which is corroborated from the research on problem solving and misconceptions that has dominated the field during the past decades. (Gabel, 1999).

Based on previous studies, Özmen (2008), summarizes the major reasons for students having difficulties in these area:

- topics are very abstract;
- words from everyday language are used but with different meanings;
- students’ lack of formal operational development and poor visualization ability;

- chemistry is described at three levels, only one of which can be readily observed.

Gabel (1999) also refers the fact that concepts are very abstract and the importance of linking new concepts to prior knowledge: “Many chemistry concepts are very abstract. If there is nothing in long-term memory to which a new concept can be related, then it will either not be stored, or it will be stored as a single entity. Hence, if something does exist to which the new concept can be related, then learning occurs. It is thought that analogies can take on this function, but in order to be effective, the students must understand the analogy and see the link between the concept being taught and the pre-existing, familiar concept in long-term memory.”

Johnstone refers to the working space (or working memory) where information is held and manipulated before being rejected or passed on for storage: “The working space has two main functions. It is the conscious part of the mind that is holding ideas and facts while it thinks about them. It is a shared holding and thinking space where new information coming through the filter consciously interacts with itself and with information drawn from long term memory store in order to “make sense” However, there is a drawback. This working space is of limited capacity.” (Johnstone, 1997). So, although the three levels are important, we have to teach them in such a way that the working space is not overloaded and the most common suggestion is to introduce macro, then micro and after that finally translate knowledge to the symbolic language of chemistry (Devetak et al., 2009).

Sirhan *et al.* (1999) (reporting to Ausubel) drives in the same direction, pointing out the importance of adapting the new knowledge to the previous one: “While appropriate knowledge and skills must be present in the mind of the learner, it is also important to recognise that they must be accessible (able to be retrieved in a meaningful form) at the time when new material is presented. It is also important that the new material must be presented in a manner consistent with the way the previous knowledge and skills have been laid down in the long term memory.”

Table 3-1 Major processes involved in the understanding of chemistry and implications for the teaching of this science.

Major process involved in understanding chemistry	Difficulties connected to the processes	Strategies suggested
• Integrate knowledge from micro, macro and symbolic domains; • Use mathematics in the context of chemistry; • Visualize chemical models and perform mental representations; • Represent and interpret chemical language.	• Only one of the levels can be readily observed, the others being quite abstract; • The quantity of information due to the learning at three levels can overload the working memory; • Lack of formal operational development and poor visualization ability of students; • Students tend to develop alternative conceptions and use algorithms to solve problems; • Words from everyday language are used but with different meanings.	• Help students visualize the concepts at all three levels and develop scientific mental models. • Put in evidence the connection between the levels • Progress from macro to micro and then to symbolic level. • Improve conceptual knowledge. • Develop students’ visual–spatial abilities. • Use external models allowing difficult internal processes to be replaced or augmented by external actions on models; • Engage students with dynamic, multirepresentational visualizations of invisible phenomena (submicroscopic representations).

3.2. Brief reference to teaching theories

Constructivism is undoubtedly a major theoretical influence in contemporary science and mathematics education (Matthews, 2002). According to constructivism the student is no longer a passive being, pure receiver of stimuli, but the constructor of his own knowledge. Learning goes through the interior of the subject and will only be significant if it is not merely imposed by the outside.

Constructivism alerts teachers to the function of prior learning and stresses the importance of understanding as a goal of science instruction, by fostering pupil engagement in lessons (Matthews, 2002). Also constructivism has made educators aware of the human dimension of science: its fallibility, its connection to culture and interests, the place of convention in scientific theory, the historicity of concepts, the complex procedures of theory appraisal, and much else (Matthews, 2002).

The current purposes for constructivism in science teaching are related to the aim of placing students in a situation where they can construct knowledge and explore alternatives, overcoming the mere assimilation of knowledge previously elaborated (Gil-Pérez et al., 2002).

Several of the authors contributing with studies concerning education in chemistry presented in previous sections, also remark the importance of constructivist principals in education. Taber emphasizes the importance of active learning of the subject: this constructivist perspective on learning applies to all science disciplines (and beyond), and is certainly not limited to chemistry (Taber, 2001). Johnstone remarks that: “Learning is not the transfer of material from the head of the teacher to the head of the learner intact. Learning is the reconstruction of material, provided by the teacher, in the mind of the learner. (Johnstone, 1997). Construction of knowledge is seen as an important feature in the learning of chemistry, as we have seen in the previous two sections, for several reasons among them the need to deal with three levels of knowledge and the abstract nature of the subject.

The role of the teacher is also considered in references since the uncommon sense of science requires competent guidance by well-informed teachers in order to help students construct concepts compatible with the ideas of scientists about the natural world (Mintzes et al., 1998). A term commonly used in constructivism when referring to teaching is "facilitating cognitive transformation" (Matthews, 2002), with implications for the role of the teacher, that is no longer associated with the classical transmission of knowledge.

The constructivist model of learning proposes that students construct their own understanding as a result of formal instruction, everyday experiences, and interactions with their surroundings, which includes their parents, peers and acquaintances (Azizoğlu et al., 2006).

So, several of the ideas and suggestions concerning the teaching of chemistry and in particular Chemical Equilibrium appear to be in syntony with the principles of constructivism: the concern with the development of student representation abilities, the worry with the use of algorithms, the concern with the overload of memory work space and the importance of adapting new information to previous knowledge. Nevertheless, references point that constructivist proposals should not be seen as direct infallible recipes. They constitute an evolution that results from years of investigation. It was soon noticed that certain alternative conceptions were resistant to instruction, even when this instruction was explicitly oriented to producing conceptual change (Gil-Pérez et al., 2002).

Piaget, who was one of the first psychologists to look at teaching, studying the way the child learns, argued that the curriculum must accompany student development. Piaget saw learning as a biological process characterized by successive periods of assimilation, accommodation and equilibration (Mintzes et al., 1998). The most critical event is considered the transition from the "concrete" to the "formal" stage, in which logical operations such as hypothetical-deductive, combinatorial, probabilistic, and reasoning operations become available. In this context, the role of the teacher is to ensure the adequacy of the learning task (Mintzes et al., 1998).

Vygotsky's base idea is that, although young children come equipped with a host of physiological and psychological dispositions that serve as the basis for distinctively human functions, their capabilities are shaped to a large extent by the cultural practices and systems of ideas of the community in which they find themselves. Children need to appropriate the conceptual resources of the pre-existing cultural world, which are transmitted to them by parents, other adults (even researchers), and peers (Nicolopoulou, 1993). "A central concept in Vygotsky 's theory of cognitive development is the "zone of proximal development" which he defines as the difference between a child's 'actual developmental level as determined by independent problem solving and the level of potential development as determined through problem solving under adult guidance or in collaboration with more capable peers.” (Nicolopoulou, 1993).

Vygotsky justifies the special role of parents and teachers as involving the systematic transmission to children of the accumulated cultural resources, including linguistic and other symbolic systems, cognitive frameworks and concrete knowledge. These resources guide children's interpretations of the world and help them to systematize the diverse physical and social phenomena they encounter. The actualization of the 'zone of proximal development' thus depends on social interaction within a shared cultural framework. This interaction can consist of both instruction and other forms of joint activity. Vygotsky further comments that a child benefits most from such interaction when it is geared appropriately to his or her level of potential development, thereby advancing actual development. (Nicolopoulou, 1993).

Bruner and Ausubel were two important authors, who, although with very personal positions, are in several aspects considered constructivists. Bruner advocated learning by the method of discovery, in which the student, guided by the teacher, must deduce the principles and laws underlying the concepts. This teaching presupposes research, observation and exploration activities. Some of the criticisms pointed out to this author are the unwanted consequences that can result from a bad orientation, the fact that it is a time consuming process and could potentiate a misconception of Science, since the student always arrives at the correct result and in the scientific method the conclusions are not so simple. According to Bruner (1960) cited by Mintzes *et al.* (1998), students should be encouraged to develop the intuitive and analytical capacities of scientists.

Ausubel argues that in order to achieve good results in learning and for it to be meaningful, teaching must be very well organized and oriented. Students need to have well-acquired prerequisites in order to adapt their knowledge. "The most important concept of Ausubel is the distinction between meaningful learning and mechanical learning (Mintzes et al., 1998). According to Ausubel, meaningful learning can be explained by a process of "subsumption", in which the new knowledge, composed of more specific (less inclusive) concepts, is linked to more general and inclusive concepts and propositions that are already part of the cognitive structure. The teacher must establish cognitive bridges, to relate the subject to the knowledge that the student already has, so that he can understand what he is learning and integrate the new knowledge into his cognitive structure. Ausubel wrote "the factor that most influences learning is what the student already knows. Find out what he knows and teach accordingly "(Mintzes et al., 1998).

To close this section let´s address two valued paradigms in science teaching: the movement of alternative conceptions and the STS (Science Technology and Society) perspective. The first is related to the development of misconceptions in students, very common in abstract themes such as the one in which this work is focused and the second seeks to make Science motivating and concepts more meaningful for students, by verifying their importance in everyday situations. According to the theory of alternative conceptions, the teacher must begin by questioning the students about the subjects in order to discover the ideas they have. Next, you should adopt methodologies that demonstrate to students the bankruptcy of their conceptions. The resistance of misconceptions could be very high and the destruction of these ideas implies a planned and engaging strategy.

The current STS movements emphasize the links between disciplinary concepts and real-world problems (Mintzes et al., 1998). According to the STS perspective, the contents should be taught aiming at an association between Science, Technology and Society. With this strategy, the student is expected to integrate theoretical knowledge into practical application contexts, such as technological applications or environmental problems in an easier way.

3.3. Learning difficulties and misconceptions in Chemical Equilibrium

From the characteristics referred in Chapter 2, we conclude that the learning of Chemical Equilibrium involves formal reasoning and the interpretation of microscopic models that imply abstraction from what is directly observable (Sarıçayır et al., 2006). Several authors develop or point to studies where Chemical Equilibrium is labelled as one of the most difficult concepts to understand (Hackling & Garnett, 1985; Huddle et al., 2000; Maskill & Cachapuz, 1989; Wilson, 1998) and one of the more challenging to teach (Banerjee, 1995; Huddle et al., 2000). Kousathana and Tsaparlis (2002) remark that Chemical Equilibrium problems are among the most important and at the same time most complex and difficult problems in general chemistry. The Chemical Equilibrium is one of the themes that propitiate the development of misconceptions, and it is verified that the most diverse learning difficulties in Chemical Equilibrium are reported over decades. In this paper, we present the most common alternative conceptions in the contents related to the Chemical Equilibrium (Azizoğlu et al., 2006; Bergquist & Heikkinen, 1990; Cheung, 2009; Hackling & Garnett, 1985; Özmen, 2008; Van Driel et al., 1999; Van Driel & Gräber, 2002), identified in studies conducted since the 1960s (Van Driel et al., 1999; Tyson et al., 1999) up to the present time (Cheung, 2009; Erdemir et al., 2000; Furió et al., 2000; Karpudewan et al., 2015; Solaz & Quílez, 2001; Van Driel & Gräber, 2002).

Students' misconceptions interfere with subsequent learning. When the students are left to connect new information into their cognitive structure these misconceptions hinder integration of the scientific knowledge. This causes weak understanding or misunderstanding of the concept (Azizoğlu et al., 2006).

During a master's dissertation, prior to this doctoral program, an extensive bibliographical review was done on misconceptions and difficulties in Chemical Equilibrium. This revision is now recovered and presented, since it was one of the base elements for the construction of the pedagogical approach to apply in the teaching of Chemical Equilibrium (Chapter 5).

Hackling and Garnett, (1985) found that most of the misconceptions are related to conceptual aspects, such as the dynamic character of Chemical Equilibrium, the rates of the forward and the backward reaction, extent versus rate of reaction, or the effect of a catalyst. This vision is in accordance with one of the difficulties verified in the learning of chemistry, pointed in last section: the importance of a solid conceptual base for students to be able to understand equilibrium. Hackling and Garnett (1985) registered the following alternative conceptions:

- The rate of the direct reaction increases as the reaction proceeds;
- There is a simple arithmetic relationship between reagent and product concentrations, such as equal concentration of both reagents or reagents and products;
- After adding a reagent, the amount of this reagent remains the same;
- When adding a reagent the rate of the reverse reaction decreases, as does increasing the temperature in an endothermic reaction, or decreasing the volume in a reaction with a greater number of moles in the products;
- When equilibrium is restored, the rates of the forward and reverse reactions are the same as at the initial equilibrium;
- Changes in volume and concentration cause changes in the value of the equilibrium constant and the temperature does not directly affect the equilibrium constant;
- A catalyst may affect differently the rate of the forward and reverse reactions.

Maskill and Cachapuz (1989) used tests based on word association to identify the ideas developed by students and found that:

- Students develop a balance-sheet view of Chemical Equilibrium (more static than dynamic);
- The idea of reversibility is understood as the possibility of moving in one direction or another, but alternately and linearly;
- Inability to relate reaction rate with the collisions theory;

- In gas phase reactions, pressure is associated with force rather than collisions between particles or their motion;
- Lack of understanding the true meaning of the term "concentration" and its influence on the equilibrium;
- The idea that the faster the reaction, the greater the quantity of products produced;
- The quantities of reagents and products are the same at equilibrium state.

Bergquist and Heikkinen (1990), situate students' alternative conceptions in four general areas of difficulty:

a) Students show difficulties with quantities of substances and concentrations:

- trying to calculate concentrations when they are already given;
- assuming that the ratio between stoichiometric coefficients is applied to product and reagent concentrations at equilibrium;
- assuming that the molar amounts are equal even when one of the reactants is in excess.

b) Students show confusion about the appearance and disappearance of material, assuming

- that concentrations vary when equilibrium is established;
- that the reaction is reversible and complete;
- that the forward reaction must be completed before the reaction in the opposite direction begins;
- that the addition of more reagent varies only the product concentration.

c) Students show confusion about the equilibrium constant:

- describing it as varying in value despite being at constant temperature;
- assuming that its value varies when changing the concentrations of reactants or products.

d) Students demonstrate misunderstanding Le Chatelier's principle by:

- trying to apply it to a system that is already in equilibrium;
- trying just to change the concentration of the added reagent;
- trying to change the concentration of all species present, except that of the added reagent;
- expressing uncertainty about how the changes in temperature, volume or pressure (including the addition of inert gases) change the equilibrium concentrations.

Banerjee (1991) carried out a study that determined the existence of alternative conceptions in Chemical Equilibrium not only in students but also in teachers. Among the alternative conceptions detected is the fact that teachers and students fail to realize that Le Chatelier's principle is limited only to qualitative information. Teachers and students demonstrate conceptual difficulties when applying reasoning too intuitive while using this principle. They also found that, in many cases, students and teachers had the idea that by lowering the temperature in an exothermic reaction, the rate of the direct reaction increases (in fact as the temperature decreases, both reactions slow down, but the most impaired is the reverse reaction that needs more energy). The problem in this case is that, once again, one is trying to apply the principle where it is no longer valid, i.e. the field of reaction rates. Banerjee (1995), also found that:

- Whenever an equilibrium constant is given, students consider that all concentrations provided (e.g. initial concentrations) are also those of equilibrium;

- Although students use the term equilibrium constant, they have difficulty understanding the existence of a balance in reactions that are virtually complete or occur to a very small extent;
- When the temperature decreases in an exothermic reaction the rate of direct reaction increases (thereby confusing extension and rate of reaction due to the attempt to misapply the Le Chatelier principle to the reaction rate);

- High values of the equilibrium constant imply very fast reactions;

- Difficulty in understanding the role of catalysts in equilibrium;
- Difficulty in interpreting the Gibbs energy equation;
- Confusion between Gibbs energy, reversibility, spontaneity and equilibrium.

Griffiths (1994) also found the prevalence of common misconceptions like:

- the rate of the forward reaction is greater than the reverse one at equilibrium;
- no reaction occurs at equilibrium;
- a catalyst affects the rates of the forward and reverse reactions differently;
- concentration of the products or reactants change with addition of a catalyzer.

Furió, Calatayud, Bárcenas and Padilla (2000) found that the functional fixation with which Le Chatelier's principle is applied leads students to often consider that adding a solid reagent is the same of adding any other. Likewise, in the inert gas additions not all influencing factors are considered, as if the addition is carried out at constant volume or pressure.

Solaz and Quílez (2001), identify a series of alternative conceptions that they associate to erroneous uses of Le Chatelier's principle:

- The addition of reagents, at constant pressure and temperature, always implies the displacement of the equilibrium towards the formation of the products;
- The addition of solids in heterogeneous equilibrium alters equilibrium;
- The addition of an inert gas to equilibrium never disturbs it, since the gas does not react;
- The addition of inert gas at constant volume and temperature increases the total pressure and this change is minimized by displacement in the direction in which there is a decrease in the total number of moles of gaseous species;

- The addition of inert gas at constant pressure and temperature disrupts equilibrium by increasing the pressure and as such the change is minimized by the displacement in the direction in which the total number of moles of gaseous species is decreased;
- The addition of an inert gas at constant pressure and temperature does not disturb the equilibrium because the volume increases but this does not affect the equilibrium because the pressure is kept constant; the mole fractions of the gases in reaction do not vary;
- The addition of inert gases, at constant pressure and temperature, in a reaction of the type A (g) $\rightleftharpoons$ B (g) + C (g) decreases the partial pressure of A, which causes a shift towards the reactants.

Van Driel and Gräber (2002) gathered alternative conceptions detected over the years in previous studies. Among the alternative conceptions assembled are many of the previously mentioned. In any case, in order to understand that these students' ideas are consistently verified in several articles, the alternative conceptions and difficulties compiled by these authors follow:

- No distinction between irreversible and reversible reactions;
- The direct reaction is completed before the reverse reaction begins;
- No distinction between speed and extension of reaction.
- The rate of the direct reaction increases over time;
- No reaction occurs during equilibrium;
- Equilibrium is seen as an oscillating pendulum;
- Compartmentalized view of equilibrium, believing that there is a left side and a right side that act independently;
- Mass and concentration mean the same for the species present in the equilibrium;
- There is a simple relationship between reagents and products at equilibrium, with the most common being the idea that at equilibrium the concentration of reagents is equal to that of products.
- Incomprehension of Le Chatelier's principle, seeking to apply it without understanding;
- Attempting to apply the Le Chatelier´s principle in situations outside the scope of this principle, such as the addition of inert gases or liquid and solid substances;

- Application of the general formulation of the Le Chatelier’s principle to changes in pressure or volume, in the same way;
- In the formation of a new equilibrium the rate of the reactions is equal to the previous equilibrium;
- When the temperature of a system is changed, evolution can be predicted without knowing whether the reaction is exothermic or endothermic;
- Students with compartmentalized vision believe that changes in equilibrium produce effects on only one side of the equation;
- The equilibrium constant changes with changes in concentration or volume;
- The equilibrium constant is independent of temperature;
- The catalyst affects, in a different way, the velocities of the direct and inverse reaction, implying changes in the value of the equilibrium constant;
- A higher value of the equilibrium constant implies a faster reaction;
- Errors in the calculation of the equilibrium constant due to lack of understanding of stoichiometry;
- No association of changes in equilibrium with changes in energy and entropy of the system.

Some misconceptions regarding Chemical Equilibrium might be the result of instruction that emphasize correct concepts without highlighting common conceptual errors. Chemistry teachers should be aware of students' prior knowledge and misconceptions. They should examine why misconceptions occur and use learning activities to eliminate misconceptions, because it is very difficult to remove misconceptions from the minds of the leaners (Erdemir et al., 2000).

The references about misconceptions presented up to this point are, in some cases, decades old, so it could be pointed out that these misconceptions are outdated and no longer represent the difficulties students face when learning Chemical Equilibrium. Nevertheless, the deepening of the review made during the master degree with some recent references shows that similar misconceptions continue to be diagnosed in students. One of this works was conducted by Özmen (2008). He verified that students had difficulties in representing and conceiving the dynamic nature of chemical phenomena, and especially those involving chemical equilibrium situations. A majority of them had inappropriate understanding of the approach to equilibrium, and they manifested serious difficulties in conceiving the shift of equilibrium and the constancy of the equilibrium constant, and they misapplied Le Chatelier's principle to explain the effects of temperature, concentration, and catalyst. "Although students took several chemistry courses during their previous schooling in order to learn various science concepts, including Chemical Equilibrium, the presence of alternative conceptions in their explanations indicates their fragmented understanding of these abstract concepts." Özmen (2008) identified the presence of 15 misconceptions and among them we can find great similarities with previous studies:

- Forward reaction goes to completion before the reverse reaction starts;
- When there are equal concentrations of substances on both sides of an equation, chemical equilibrium has been reached;
- The rate of forward reaction is greater than the reverse reaction rate;
- Equilibrium reactions go on until all the reactants are consumed;
- At equilibrium, no reaction occurs;
- Le Chatelier's principle can be applied in the initial state before the reaction has reached equilibrium;
- When a substance is added to equilibrium mixture, equilibrium will shift to the side of addition;
- When the temperature is changed, whether the reaction is endothermic or exothermic does not affect the direction of the equilibrium shift;
- When the temperature is increased, more products form;
- An increase in temperature always increases the numerical value of K_{eq};
- Equilibrium constant, K_{eq}, will increase with increasing temperature in an exothermic reaction;
- When more products are added to an equilibrium system at constant temperature, K_{eq} will increase;
- The numerical value of K_{eq} changes with variations in the amounts of reactants or products;
- Le Chatelier's principle can be applied in all systems, including heterogeneous equilibrium systems;
- Increasing the amount of a solid ionic substance that is at equilibrium causes more dissolved ions to be produced.

Cheung (2009) also developed a study in misconceptions on Chemical Equilibrium concluding that the most important implications of the research have to do with curriculum content and chemistry teacher education: Secondary students find Chemical Equilibrium very difficult not only because the concepts of Chemical Equilibrium are abstract but also because there are problems in the selection of curriculum content. Cheung particularly criticizes the use of Le Chatelier's principle (LCP): "The inclusion of LCP in the school chemistry curriculum does not meet two important criteria for selecting curriculum content: significance and validity. Significance refers to the extent to which the selected content is essential to the topic under study and enables students to engage in learning in meaningful ways. Validity is concerned about the accuracy of the content. LCP does not open the door of learning opportunities for students; rather it deters their meaningful learning of chemistry because application of LCP may result in inaccurate predictions." (Cheung, 2009). Cheung suggests replacing Le Chatelier's principle for reaction quotient and a simplified version of the Van't Hoff equation, for secondary chemistry courses. Other authors also found that The simplistic definition of LCP is likely to have caused serious errors in its application to equilibrium systems (Karpudewan et al., 2015).

Table 3.2 organizes the alternative conceptions and difficulties mentioned above, seeking to constitute a synthesis, in order to better interpret and distinguish the ideas identified.

Table 3-2 Synthesis of difficulties and misconceptions reported in the learning of Chemical Equilibrium.

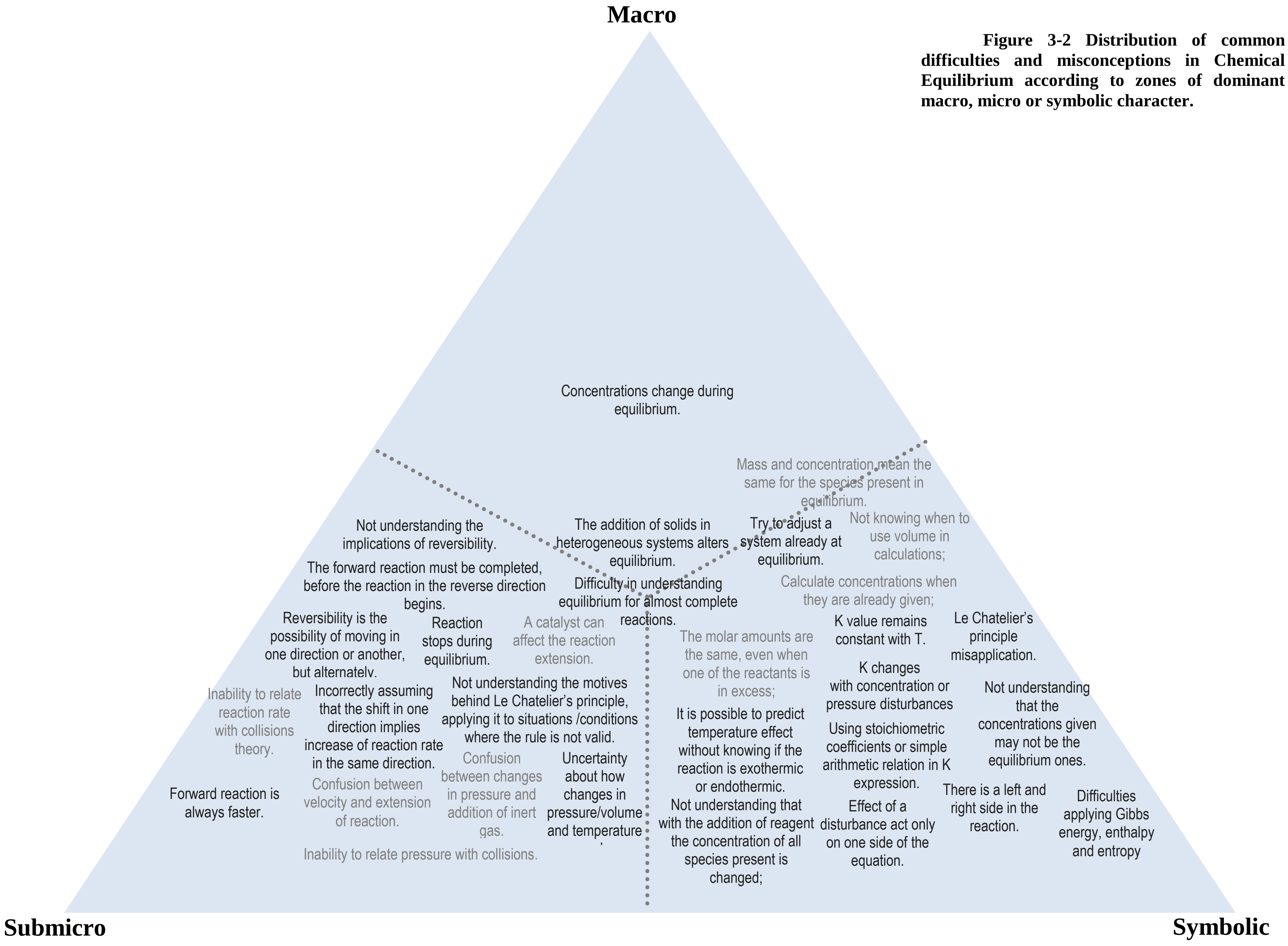
Topics		Alternative conceptions and general difficulties
Reversible Reactions		- No distinction is made between the implications of a reaction being reversible or irreversible; - The forward reaction must be completed, before the reaction in the reverse direction begins; - Reversibility is the possibility of moving in one direction or another, but alternately and linearly.
Equilibrium quantification	Related Calculations	- Calculate concentrations when they are already given; - Not knowing when to use volume in calculations; - The molar amounts are the same, even when one of the reactants is in excess; - Mass and concentration mean the same for the species present in equilibrium.
	Equilibrium constant	- Its value remains with changes of temperature; - Its value varies with changing the concentrations of reagents or products; - There is a simple arithmetic relationship between reagent and product concentrations, such as equal concentration of both reactants or reagents and products; - The ratio between the stoichiometric coefficients applies at equilibrium concentrations; - Whenever an equilibrium constant is given, the given concentrations are also those of equilibrium; - Concentrations vary when equilibrium is established; - Although students use the term equilibrium constant, they have difficulty understanding the existence of a balance in reactions that are virtually complete or occur to very small extent.
Equilibrium disturbance	Changes in Reagent and Product Amounts	- With the addition of more reagent only the product concentration varies; - With the addition of reagent only the concentration of the added reagent changes; - With the addition of reagent the concentration of all species present is changed, except those of the added reagent; - After adding a reagent, the amount of this reagent remains the same; - The addition of reagents, at constant pressure and temperature, always implies the displacement of the equilibrium towards the formation of products; - The system shifts in the direction of an added substance.
	Changes in Pressure / Volume	- Uncertainty about how the variation of volume or pressure changes the equilibrium concentrations; - Confusion of this situation with the pressure change by addition of inert gas.
	Changes in Temperature	- When the temperature of a system is changed, the evolution can be predicted without knowing whether the reaction is exothermic or endothermic; - Uncertainty about how temperature variation changes equilibrium concentrations; - When the temperature is increased, more products form; - An increase in temperature always increases the numerical value of K_{eq}; - Equilibrium constant, K_{eq}, will increase with increasing temperature in an exothermic reaction.
	Other disturbances	- The addition of an inert gas to the Chemical Equilibrium never disturbs it, since there is no reaction; - Addition of inert gas, at constant volume and temperature, increases the total pressure and this change is minimized by the displacement in the direction in which the number of moles is decreased; - The addition of an inert gas at constant pressure and temperature does not disturb the equilibrium; - The addition of inert gases at constant pressure and temperature in a type $A(g) \rightleftharpoons B(g) + C(g)$ reaction decreases the partial pressure of A, which causes a shift towards the reactants; - The addition of inert gas at constant pressure and temperature disrupts equilibrium, increasing the pressure, as such the change is minimized by the displacement in the direction in which the number of moles is decreased; - The addition of solids in heterogeneous equilibrium alters equilibrium.
	General disturbances	- Attempt to adjust a system that is already in equilibrium; - Changes in equilibrium have effects only on one side of the equation.

Topics		Alternative conceptions and general difficulties
Le Chatelier's Principle		- Application to the addition of inert gases, liquid and solid substances; - Application to changes in the extent and speed of the reaction simultaneously; - Application to changes of volume without understanding that it's the change of pressure that the system seeks to counteract; - Misunderstanding the principle significantly, seeking to apply it with no understanding - Le Chatelier's principle can be applied in the initial state before the reaction has reached equilibrium.
Dynamic Equilibrium		- No reaction occurs during equilibrium; - Oscillating vision of Chemical Equilibrium (more static than dynamic); - There is a left side and a right side in equilibrium, which act independently; - Difficulty in understanding the equilibrium in reactions that are virtually complete or that practically do not occur.
Kinetics and Equilibrium	Catalysts	- A catalyst may differently affect the rate of the forward and reverse reactions; - The catalyst affects in a different way the velocities of the direct and inverse reaction implying changes in the value of the equilibrium constant.
	Disturbances to Equilibrium	- When the temperature decreases in an exothermic reaction, the rate of the direct reaction increases; - When adding a reactant, the rate of the reverse reaction decreases, as does increasing the temperature in an endothermic reaction, or decreasing the volume in a reaction with a greater number of moles in the products.
	General ideas	- Inability to relate reaction rate to collisions theory; - Pressure is associated with force rather than collisions between particles or their motion; - The faster the reaction, the greater the amount of product produced; - A higher value of the equilibrium constant implies a faster reaction; - The rate of the direct reaction increases over time; - When equilibrium is restored, the rates of the forward and reverse reactions are the same as at initial equilibrium; - The rate of forward reaction is greater than the reverse reaction rate.
Thermodynamics		- Not associating changes in equilibrium with changes in energy and entropy of the system; - Difficulty in interpreting the Gibbs energy equation; - Confusion between Gibbs energy, reversibility, spontaneity and balance.

We have made the exercise of situating the difficulties/misconceptions reported in Table 3.2 according to the macro, micro and symbolic zones in Chemical Equilibrium knowledge space. In some cases we have combined similar misconceptions in only one more embracing sentence. To elaborate the triangle, we analysed in which of the three dominant zones resides the cause for each difficulty/misconception. Let´s pick for instance the misconception: “There is a left side and a right side in equilibrium, which act independently”, we think this idea is directly connected with the misinterpretation of the symbolism used in chemical equations where there is the “side” of the reagents and the “side” of the products and so we have placed it in the symbolic domain but also with some contribution from the micro domain, since a good understanding of dynamic equilibrium could avoid this idea.

Interpreting the resulting triangle (Figure 3.2), we verify (without much surprise, according to previously exposed ideas such as the labelling of micro and symbolic levels as abstract) that most of the misconceptions are related to absent/incorrect knowledge in the micro and symbolic levels.

Figure 3-2 Distribution of common difficulties and misconceptions in Chemical Equilibrium according to zones of dominant macro, micro or symbolic character.



3.4. Epistemology of Science's Input

The Epistemology of Science can help us reflect on the evolution in the knowledge about chemical reactions along the centuries, which, in turn, can contribute to identify causes for students' difficulties in the learning of this thematic and especially in Chemical Equilibrium. In this section we make a brief incursion trough Epistemology of Science, applying the ideas of some relevant personalities in that field to chemistry and in particular to Chemical Equilibrium.

In chapter 2 we have seen that the microscopic domain is considered an essential feature of the knowledge in chemistry. The question of atomic structure is usually approached from an evolutionary point of view, focusing on history and sequential achievements. This theme is considered the "sine qua non" of education in chemistry (Tsaparlis, 1997).

From ancient Greece, philosophers deal with the understanding of the constitution of matter, seeking to arrive at a unifying principle on this subject (Tsaparlis, 1997). The first ideas about the discontinuous nature of matter are attributed to Leucippus (500 BC) and Democritus (468-370 BCE) (Tsaparlis, 1997; Chang, 2005). These philosophers considered that dividing matter to the smallest unit would arrive at an indivisible particle, which they designated by atom (Tsaparlis, 1997). The atoms would be indestructible and varied in weight, shape and size, thus justifying the existence of different materials (Tsaparlis, 1997). This discussion was only consistently resumed around 1800 (Tsaparlis, 1997), when Dalton's atomic theory was published. This English physicist, based on the studies of previous scientists, proposed in 1808 his atomic theory, whose lines of force are as follows (Chang, 2005):

- all matter is composed of atoms;
- atoms are indivisible;
- atoms do not transform into one another;
- atoms cannot be created or destroyed;
- atoms of different elements are different from each other;
- the whole chemical reaction consists of the union or separation of atoms.

This theory supported Lavoisier's Law, previously established, according to which "nothing is lost, nothing is created and everything is transformed" (Chang, 2005). It is attributed to the English physicist, Thomson the discovery of the electron, marking the entry into the universe of subatomic particles and putting an end to the idea of an indivisible atom. Thomson sought evidence for Dalton's atomistic theory (Videira, 1993) and found that cathode rays were particles of very small negatively charged dimensions: electrons (Chang, 2005; Reger et al., 1997). It was concluded that these particles exist in the interior of the atom to counteract the model of Dalton's rigid sphere, replacing it with the "plum pudding" model in 1887. In this model, negatively charged electrons were scattered randomly by a sphere of positive mass (Chang, 2005). There followed a phase in which the knowledge of new radiations “exploded”. Rutherford formulated a new model for the constitution of the atom: the planetary model. In this model the electrons moved around a nucleus that had a positive charge, small dimension and concentrated almost the entire mass of the atom. On the basis of these evidences, Rutherford concluded that an atom had a lot of free space, since most of the particles cross the gold leaf (Chang, 2005) At the turn of the twentieth century, several scientists began to recognize that classical mechanics was not enough to explain phenomena related to the atomic universe. Several doubts were posed in relation to Rutherford's model, for example explanations for the fact that particles with charges of the same signal concentrate in the nucleus of the atom. On the other hand, Rutherford's model posed a problem. According to the laws of electromagnetism established at the time an electric charge loses energy in the form of radiation as it moves which leads to its collapse to the nucleus. New data, namely discoveries about light, demonstrated the need to appeal to new types of thinking, such as the particle wave duality. The initial step was given by Planck in 1900, when he stated that energy is absorbed and emitted in discrete quantities, introducing the term "quanta" of energy. Although he came to this conclusion by statistical reasoning, Planck failed to give a good justification for considering quantized energy (Chang, 2005). Experiments on the photoelectric effect came to support the theory defended by Planck. In 1905, Einstein would come up with a quantitative explanation for this phenomenon, which led to the acceptance of energy quantification ideas. This was an important step for the formulation of the first model of the atom taking into account the quantization of energy: the Bohr model. This model also provided an explanation for the spectroscopic results that were beginning to emerge (Chang, 2005). According to his theory, the hydrogen atom has certain stable states of energy and is associated with stationary circular orbits, described by the electron. Bohr thus elaborated a quantum theory, where for the first time it points to the existence of discontinuous levels of energy in the atom (Chang, 2005).

Heisenberg, around 1926, sought to develop theory through what is observable, like the light emitted and absorbed by matter, and after a few years of work he was able to base his ideas on mathematical bases, designating the new theory by quantum mechanics. Heisenberg stated that since the electron is so small, it is not possible to determine its position and linear momentum at the same time, so it proposed to change the idea of orbits by the idea of probability of finding an electron. More contributions were given and Bohr's model was eventually abandoned: instead of orbits, there were zones of greater or lesser probability of finding electrons. In 1927, the Austrian physicist, Erwin Schrödinder, formulated, by pure mathematical intuition, a wave equation valid for the electron of the hydrogen atom. Since it was fully adapted to experimental observations, his equation provided a great development of quantum mechanics in the following years (Chang, 2005). The new theory was a hot topic for discussion at the Solvay conference in 1927. In 1934, Einstein acknowledged that the theory he himself had helped build was the best model found to date to describe the atom's statistical behaviour. Nevertheless, he considered that the theory was not yet complete, having dedicated the last years of its life in the attempt to deepen it. In the 1960s intense research has revealed that particles considered to be basic until then are actually composed.

Kuhn argued that the change in science occurred for scientific and non-scientific reasons (philosophical beliefs, etc.) diverging from scientist to scientist. According to Kuhn, a new paradigm should be able to solve the problems of the previous one but this does not mean that it is closer to the truth. It is simply a dogma that at the moment unites scientists. The triumph of a new paradigm may be due to a variety of factors: its ability to explain controversial facts, its usefulness in solving problems, appropriate predictions, and the aura and prestige of scientists (Chalmers, 2000). This view is compatible with references pointing that Dalton's prestige made his ideas prevail unchanged for about 50 years (Chalmers, 2000).

In the context of chemical reactions it is also arguable that the affinities theory had several important personalities as defenders, leading this theory to persist for a long time. It was the acceptance of the atomic theory, in the terms described in this section, which definitely led to a different road in the explanation of chemical reactions, incurring trough kinetics and leaving apart the mechanical view instituted at the time. The notion that chemistry, as well as other sciences, is in constant evolution, for which contribute scientific and non-scientific causes is an important feature for students to understand models. “Among science research educators there is an emergent consensus about the incorporation of the history of science into the curriculum. Historical knowledge of chemistry may contribute to the understanding by the teachers of students’ difficulties and alternative conceptions, enabling them to address the issues of instruction; that is, to formulate general chemical problems as well as didactic learning sequences that eventually may facilitate the apprenticeship of the related concepts.” (Quílez, 2004).

Kuhn referred by Oki (2007) stated that it was possible for a community of chemists to work with instruments based on the existence of atoms, such as chemical combinations, but not all members believing in their existence. It was agreed that atoms and molecules were necessary to chemistry, even considering them as hypothetical (Oki, 2007). In this case the atom was the dogma that united the chemists for its usefulness in this historical context, giving chemistry an object of study. This idea in accordance with a position often stated that “Science seeks to provide explanations for natural phenomena: to describe the causes that lead to those particular effects in which scientists are interested. However, ‘phenomena’ are not ready – made: we impose our ideas of what might be important on the complexity of the natural world” (Gilbert, 2005). We think it is important that students understand this purpose, so that they realize that when dealing with the micro world in chemistry we are using ideas to better explain what happens in the macro world, models that were constructed identifying which is essential for the phenomena in the complexity of the natural world. Most of the students are able to reason in macroscopic terms, but only a few relate the observed phenomena to their corpuscular conceptions (Van Driel et al., 1999).

According to Lakatos, scientists work in scientific research programs, which have an irrefutable core to which the scientific community adheres and advocate for new evidence - enhancements that reinforce a protective belt of this program. The refutation of a program is a slow process which occurs mainly due to difficulties coming from experimental observation that weaken the protective belt and attack it, so that the program of scientific investigation enters in degeneration. However, the transition may also be somewhat driven by external factors that give more or less relevance to the difficulties encountered (Chalmers, 2000; Lucena, 2005). As exposed in chapter 2 abnormalities in the theory of affinity started to arise from experiences, exposed by Bertholet among others, leading to a slow destruction of its protective belt. When the abnormalities have reached the nucleus of the theory, then it can no longer prevail among the scientific community. Some students conceptualise chemical equilibrium as a product of opposing forces, which leads to a static view, as a prevalence of mechanical ideas applied to chemical equilibrium (Niaz, 1998). As already referred in previous section the alternative conceptions students develop, usually based on common sense, are very resistant and tend to persist unless a strategy capable of conceptual change. Niaz (1995) recommends that the teacher seeks the "hard core" of student ideas (alluding to the epistemology of Lakatos). This core of knowledge is more resistant to change than ideas found in the protective belt. The destruction of alternative conceptions implies the direct confrontation of the student with the inability of his or her hard core of ideas to explain a given phenomenon (Niaz, 1995).

We can also apply Lakatos' epistemology to the abandonment of Dalton´s model of the atom. More and more contributions were made in the field of atomic structure, and there were no new evidences supporting that the atoms are made up of spheres. Dalton's model was eventually abandoned by Thomson's model, which solved the problems of the previous one, in light of the new experimental evidence. It is also verified that Thomson had formulated hypotheses to "conquer" chemists with slightly different visions, but compatible with the hard core of his proposal, being seen as a form of negative protective heuristic of the hard core (Niaz, 1998). Lakatos provided a dynamic picture of science in which each refuted theory has relative merit. In Chemical Equilibrium education it is defended that the use Dalton's model of the atom is a good approximation to help students' visualize the events during chemical reactions: "For beginners it is possible to catch the idea of structural models on the basis of Dalton… The main point should be the possibility that students can develop not only knowledge but also images…" (Barke & Wirbs, 2002).

Kuhn, in his theory of scientific revolutions, introduces the notion of paradigm and considers that it unifies the conceptual unit of language and methodology. Then the scientist works for the paradigm (his dogma) to differentiate and broaden it. When anomalies arise and difficulties get out of hand, someone who lives in crisis and is creative suggests a new paradigm different from the previous one. This will have to be able to solve more problems but it does not mean that it is closer to the truth. Observation is important but it is the point of arrival - one tries to observe what the paradigm points to (Chalmers, 2000; Lucena, 2005). This can explain why Van't Hoff developed both an incursion trough kinetics and thermodynamics in trying to explain chemical reactions and, according to Kuhn, these theories are not measurable since they are based on different assumptions. For Kuhn the importance of an issue like Dalton's atomism depends on the paradigm of the theorist who "sees" it. The way a scientist sees a particular aspect of the world is guided by the paradigm to which it is attached. Kuhn argues that proponents of rival paradigms "live in different worlds". So, once again these ideas show the importance of representation and the guidance of the students in the construction of the scientific models in order to avoid the development of rival paradigms in the mind of the student.

From this section review, we can add the following recommendations to the teaching of chemistry:

- Knowledge about the History of Chemistry can help understand students' misconceptions and minimize them;

- It is important for students to understand the explanatory power of the sub-micro level and the character of the model that this level retains – the micro world in chemistry represents the ideas that better explain what happens in the macro world, models that were constructed identifying what is essential for the phenomena in the complexity of the natural world;

- The destruction of alternative conceptions implies the direct confrontation of the student with the inability of his or her hard core of ideas to explain a given phenomenon;

- The importance of representation and the guidance of the students in the construction of the scientific models in order to avoid the development of rival paradigms in the mind of the student.

3.5. Chemical Equilibrium in the Portuguese Chemistry Curriculum

In the current curriculum of chemistry, CE is taught in the 11th grade. This means that students should reach this stage with an age around sixteen to seventeen years old. In Portugal, Chemistry and Physics are taught together in a subject named Physics-Chemistry from 7th grade to 11th grade. Only in the last year of high school studies (12th) are these sciences taught as independent subjects for students in the scientific-technologic field of studies, whom can choose between physics, chemistry, biology and geology among other optional subjects.

The syllabus for the discipline of Physics-Chemistry for both the 10th and the 11th grades was recently reformulated (2014) and new directives and goals were defined for teaching Chemical Equilibrium as well as other thematics. The contents were selected with the aim of maintaining the essential aspects of the previous programs (Physics and Chemistry A from the 10th year, homologated in 2001, and from the 11th year, homologated in 2003) (Martins et al., 2003).

As general goals for the subject the document refers (Fiolhais et al., 2014):

- To provide students with a solid base of skills and knowledge of Physics and Chemistry, and science values that allow them to distinguish scientific from nonscientific claims and communicate in science by questioning, investigating and concluding.

- To promote the recognition of the importance of physics and chemistry in the understanding of the natural world, in the description, explanation and prediction of its multiple phenomena, as well as in technological development and in the quality of life in society.

- To contribute to the increase of scientific knowledge necessary for the continuation of studies and for a reasoned choice of the area of these studies.

- In order to achieve these goals, the general aims of the discipline are defined as:

- Consolidate, deepen and extend knowledge through the understanding of concepts, laws and theories that describe, explain, and predict phenomena.

- Develop habits and abilities inherent to scientific work: observation, research of information, experimentation, abstraction, generalization, prediction, critical spirit, resolution of problems and communication of ideas and results in written and oral forms.

- Develop skills to recognize, interpret and produce representations of the scientific information and learning outcomes: reports, diagrams, graphs, tables, equations, models and computational simulations.

- Emphasize how scientific knowledge is constructed, validated and transmitted by the scientific community.

From the goals defined we can see that there is a concern about scientific literacy of students and on the application of the knowledge in contexts related to technology and society, in harmony with STS perspective. Also the authors of the program make some other considerations in accordance with the ideas presented in previous sections of this dissertation, like the evocation of situations in the history of science to allow students to understand the way in which knowledge has been constructed or the fact that this discipline, by its very nature, often uses mathematical methods. Nevertheless, especially important in the context of our work is the recognition that one of the aims of the subject is to develop abilities inherent to scientific work, where abstraction is directly referred among other processes. The importance of producing representations is also referred and related with the use of computational simulations.

In what concerns specifically to Chemical Equilibrium, the thematic is divided into two subdomains, each one embracing several concepts:

Quantitative aspects of chemical reactions

(7 lessons)

General objective

To understand the quantitative relationships in chemical reactions and to apply them in determining the efficiency of these reactions.

Contents

Chemical reactions: chemical equations and stoichiometric ratios
Limiting reagent and excess reagent
Degree of purity of a sample
Yield of a chemical reaction
Atomic economy and green chemistry

- Laboratorial activity: Synthesis of acetylsalicylic acid

Chemical equilibrium and extent of chemical reactions

(8 lessons)

General Objective

Recognize the occurrence of incomplete chemical reactions and chemical equilibrium reactions, as well as use the Le Chatelier’s Principle to predict the evolution of chemical systems.

Contents

Incomplete reactions and chemical equilibrium:
Reverse reactions and chemical equilibrium
Chemical equilibrium
Extension of chemical reactions:
Equilibrium constant using concentrations
Quotient of reaction
Factors that alter the chemical equilibrium:
Le Chatelier's principle
Chemical equilibrium and optimization of chemical reactions

- Laboratorial activity: Effect of concentration on chemical equilibrium

Guidelines and suggestions are also presented for both subdomains:

Quantitative aspects of chemical reactions

The quantitative aspects of some historically relevant chemical synthesis reactions may be a context for the introduction of these contents. The quantitative aspects of the reactions can be approached, for example, starting from the chemical industry. In the domain of chemical equations it is intended to increase the learning from previous years, and it may include equations in the ionic form. Atom economy must emerge in the context of "green chemistry" to emphasize that in the case of chemical reactions, it is possible to introduce modifications aimed at saving energy and / or atoms. These aspects can be discussed with students from a sustainability point of view. It is suggested the writing of chemical equations using Lewis structures, emphasizing the molecular character.

Chemical equilibrium and extent of chemical reactions

The systems to be studied in this subdomain must be homogeneous, gaseous or aqueous. For quantitative aspects of chemical equilibrium, cases in which only the initial composition of the system is reported should be excluded. Computational simulations can be a useful tool to visualize the dynamic nature of chemical equilibrium by providing graphical representations of the evolution of reagent and product concentrations over time. These simulations will also help students recognize that a chemical system can have, at the same temperature, an infinity of states of equilibrium with the same equilibrium constant. It should be noted that the equilibrium constant always assumes a finite value (neither null nor infinite, although it may have a very low or very high value). Computational simulations may also help to understand the evolution of chemical systems resulting from perturbations to chemical equilibrium, with the advantage of being able to explore what happens microscopically in these cases, reinforcing the idea of the dynamic nature of chemical equilibrium.

The program also defines a series of specific aims for each thematic: "They identify the essential learning to be done by students ... highlighting what in the program must be the primary object of teaching." (Fiolhais et al., 2014). According to the authors these aims provide the framework for an internal and external evaluation, in particular for the national examinations, guide the teacher's action in the planning of teaching and production of materials and facilitate the self-assessment process by the student. Next we present the aims for Chemical Equilibrium.

Quantitative aspects of chemical reactions

1.1 Interpret the meaning of the chemical equations in terms of quantity of matter and the relation to the conservation of mass (Lavoisier's Law).

1.2 Perform stoichiometric calculations based on chemical equations.

1.3 Identify limiting reagent and excess reagent in a chemical reaction.

1.4 Interpret the degree of purity of a sample.

1.5 Indicate that the reagents may have different degrees of purity and that they should be chosen according to the purpose of use and cost.

1.6 Distinguish complete and incomplete reactions.

1.7 Carry out stoichiometric calculations involving limiting / excess reagent, reaction yield and reagent purity.

1.8 Associate "atomic economy" with the ratio of the mass of reactant atoms that are incorporated into the desired product and the total mass of atoms in the reactants, expressed as a percentage.

1.9 Compare chemical reactions from the point of view of green chemistry taking into account several factors such as: atomic economy, reduction of residues, unwanted products, choice of reagents and less polluting processes.

State of equilibrium and extent of chemical reactions

2.1 Interpret the occurrence of incomplete chemical reactions on a molecular basis: simultaneous occurrence of direct and inverse reactions.

2.2 Associate a state of chemical equilibrium with any state of a closed system in which, macroscopically, there are no variations of physical and chemical properties.

2.3 Interpret graphs that show the variation of the concentration (or amount of matter) as a function of time, for each of the components of the reaction mixture, and of the evolution with time of the velocity of the direct and inverse reactions.

2.4 Associate a homogeneous chemical equilibrium with the equilibrium state that occurs in a reaction mixture in a single phase.

2.5 Identify homogeneous equilibria in different contexts, for example the ammonia synthesis reaction.

2.6 Write mathematical expressions that translate the equilibrium constant using concentrations.

2.7 To conclude, from concentration values, that the value of the equilibrium constant is the same for all equilibrium states of a chemical system, at the same temperature.

2.8 Relate the extent of a reaction at a certain temperature to the equilibrium constant of that reaction at that temperature.

2.9 To conclude, from equilibrium concentration values, that the equilibrium constant value for a chemical reaction depends on the temperature.

2.10 Relate the value of the equilibrium constant of the direct reaction to that of the equilibrium constant of the inverse reaction.

2.11 Distinguish between equilibrium constant and quotient of the reaction in non-equilibrium situations.

2.12 Predict the dominant direction of the reaction based on the comparison of the value of the reaction quotient at a given instant with the equilibrium constant of the chemical reaction at the reaction temperature.

2.13 Apply expressions of the equilibrium constant and the quotient of the reaction in the resolution of questions involving calculations.

2.14 Indicate the factors that can change the equilibrium state of a reaction mixture (pressure, gaseous systems, temperature and concentration).

2.15 Interpret the effect of varying the concentration of a reagent or product on an initially at equilibrium system by comparing the reaction quotient with the equilibrium constant at constant temperature.

2.16 Identify Le Chatelier's Principle as a rule that allows the prediction of the evolution of a chemical system when there is variation of one of the factors that can affect the state of equilibrium - concentration, pressure, volume or temperature.

2.17 Apply the Le Chatelier’s Principle to the synthesis of ammonia and other industrial processes and justify aspects of compromise related to temperature, pressure and use of catalysts.

From the content of the syllabus in what concerns to Chemical Equilibrium, we would like to remark that:

- It is clearly recommended that Chemical Equilibrium should be taught making use of computational simulations, recognizing them a key resource to help visualization and mental modelling in Chemical Equilibrium;

- The importance given to the microscopic level is present in sentences like: simulations bring “the advantage of being able to explore what happens microscopically in these cases, reinforcing the idea of the dynamic nature of chemical equilibrium”; nevertheless, no other microscopic considerations are made or proposed along the guidelines for approaching CE teaching. Explanations for equilibrium displacement based on kinetic-corpuscular theory are left apart. So, it can be extrapolated that the intention of using the micro level of knowledge resides in demonstrating dynamic equilibrium, avoiding misconceptions like “the reaction stops during equilibrium” or “reactions occur in direct and reverse direction alternately”, without the explicit intention of using microscopic considerations when explaining equilibrium disturbances.

- Le Chatelier’s principle, that was recognized in previous sections to have several problems and opposing ”voices” to its use in teaching (Cheung, 2009; Tyson et al., 1999; Allsop & George, 1984), is chosen as the core strategy to analyze shifts in equilibrium state. Cheung (2009) denoted this tendency in other courses including some cases where Le Chatelier’s principle is the only approach.

- As expected, no thermodynamics is involved whatsoever in the approach of chemical equilibrium. Instead, in other theme guidelines, it is directly suggested not to introduce the concept of entropy. Chemical equilibrium is also not classified as a minimal state of energy. The use of K and Q to analyze equilibrium establishment and displacement is proposed, an idea presented in literature many years ago and that continues to be the common approach in secondary level: equilibrium law can be used to describe the course of reaction and does not require familiarity with thermodynamics (McLean, 1938).

After reviewing the current portuguese syllabus of chemistry, we can reformulate the triangle presented in Chapter 2, to include only the concepts involved in the teaching of Chemical Equilibrium according to these directives (Figure 3.3). The same notion from Chapter 2 was used, appearing in grey the concepts that constitute previous knowledge.

Gabel (1993) referred that: “using an equilateral triangle with a level at each vertex, any point within the triangle can represent the percentage of time allocated to using a given level in the teaching of chemistry”. As Johnstone has pointed out, at the present time most chemistry courses are taught at the symbolic level with little emphasis on the microscopic and the macroscopic levels.” In our triangle we notice this tendency too, since great relevance is given to the quantitative analyses using the expression of the equilibrium constant or Le Chatelier’s principle. The references to dynamic equilibrium and the contextualization with industry and real life events are the key points to include micro and macro levels respectively.

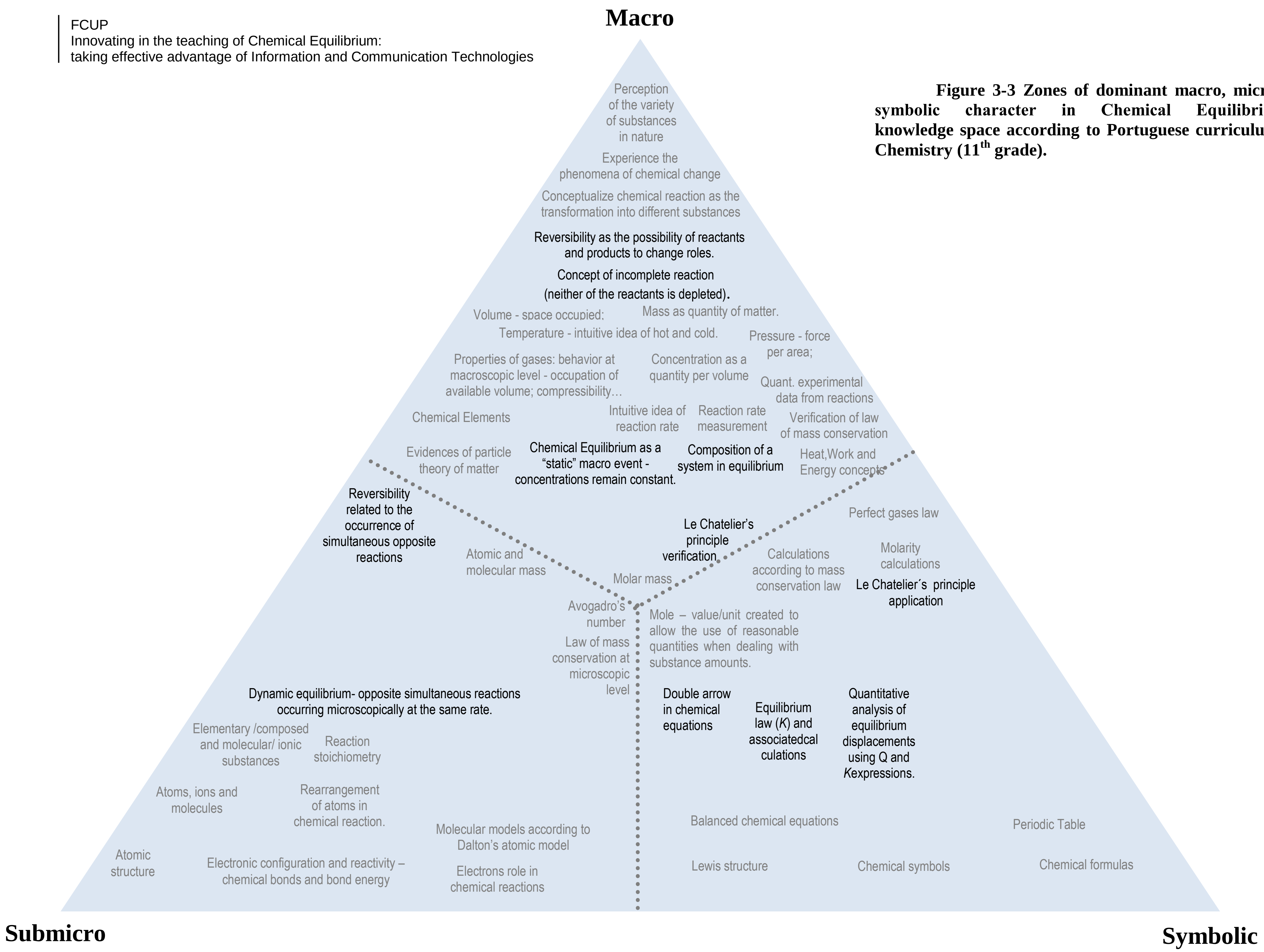


Figure 3-3 Zones of dominant macro, micro or symbolic character in Chemical Equilibrium’s knowledge space according to Portuguese curriculum of Chemistry (11th grade).

Chapter 4 - Technologic Dimension: ICT potential for the teaching of Chemical Equilibrium

4.1. Brief reference to ICT in Science Education

Currently, the diversity of computer applications with different functionalities is immense. Almost all computational products are capable of constituting educational resources. The computer makes it possible to provide a set of different media (text, sound, still and animated image, video) in a single presentation technology, and this type of integration is usually called multimedia. If we make the association with the Internet and the tools of online communication, the interaction with the user is amplified (Paiva, 2007), since the joint use of these media implies constant choices and continuous actions of selection and organization of the information collected (Fonseca, 2006).

The potential of the communication tools can also be used to facilitate collaborative learning (Renzi & Klobas, 2000); communication with science teachers and students is an obvious way of using the internet; another is to communicate with scientists (Mintzes et al., 1998); some of the software enables connections between the most abstract representations used by scientists and the representations that are familiar to the students (Mintzes et al., 1998). ICT offer the possibility of students creating, by themselves, objects or artefacts and publish their work (Mintzes et al., 1998). We can find associations between these considerations and active learning, rated according to the principles of constructivism.

The representation of scientific models is among the more valued aspects regarding the potential of computers for the teaching of sciences (Mintzes et al., 1998; Russell et al., 1997, Sandberg & Belamy, 2003; Sarıçayır et al., 2006; Sprague et al., 2005). Resources related to representation include computational simulations, software where students create their own artifacts, allowing connections between the more abstract representations used by scientists and their familiar representations (Mintzes et al., 1998) and sensors coupled to digital analyzers that can make the scientific representation of natural phenomena more intuitive (Mintzes et al., 1998). Nacheva-Skopalik and Koleva, 2012 point that novel innovative methods of training are to be introduced relying heavily on ICT in order to reduce difficulties in chemistry. ICT is considered a way to enhance the students' interest and to stimulate the active learning process concerning chemistry.

Much has been written about the present School challenge of adapting itself to the demands of the information society (Aviram, 2000; Pinto, 2002; Sinka, 2006). More recent references indicate that school change is taking place although still at a preliminary stage (Balanskat, 2006 cited by Aviram, 2009). However, the recognition of the need to modernize education and the importance of the integration of ICT in this process seems to be already a given in the last few years (Mintzes et al., 1998; Paiva, 2007; Rosa, 2000). The role of the teacher as mediator in this process of use of ICT in science education is also highlighted (Paiva, 2007).

The use of computational resources in education is favored by the development of new technologies of representation / interaction, dissemination of Web 2.0 and better technological equipping of the schools in the last years (Weigold & Treise, 2004). Another important factor is the increase in the time of permanence of the young people in the computer and online, imposing the Internet as a means of informal education of the sciences (Weigold & Treise, 2004).

There is an interest today in the adolescent approach to Websites about Science (Weigold & Treise, 2004). In a bidirectional relationship, websites can be useful to young people and simultaneously promote the public image of science. In the first hypothesis, they constitute an informal teaching medium, to support the accomplishment of the school tasks, contributing to the scientific literacy. In the second case, they can promote the development of positive attitudes towards science (Weigold & Treise, 2004).

Informal learning is traditionally associated with museums, exhibitions, science centres and television. However, Weigold & Treise (2004) argue that websites can have almost unlimited potential in this area, taking into account the characteristics that make them attractive to young people. Christensen (2007) and Çimer (2007) share the view that the dissemination of science implies a multiplatform effort.

Weigold and Treise (2004) point to the elements of added value in the "call" of the young people to science websites: entertainment/interactivity; control; content construction by the student (Web 2.0); communication; the linking of information with everyday life and the realistic modelling of phenomena. These authors also highlight the role of the teacher as the "mediator" of the audience of science sites. There is also the opportunity to complement the school curriculum with the websites, which calls for the creation of curriculum-friendly Websites.

The presence of interpretable graphical information is a relevant factor in the selection of pages on which adolescents stay longer (Christensen, 2007). Weigold and Treise (2004) argue that simulations should be more widely used on science websites and that, “appropriately constructed, documented, and targeted, simulations can provide teens with inexpensive yet sophisticated “laboratories,” in which to be participants in discovering the wonders of science”. Uploading the simulations online is an enrichment factor because the motivation to explore them is greater when other users do it simultaneously. Allowing cross-user collaboration is another interesting facet for this feature. “At present very few science sites make extensive use of simulations. And while some excellent ones exist, they fall far short of what we have proposed for allowing extensive teacher involvement and Web-based collaboration” (Weigold & Treise, 2004).

By making teenagers an active participant in science, Websites allow the transposition of "passive memorization" into "active engagement" in the learning process (Weigold & Treise, 2004).

Information has never been so accessible. However, the amount of available information far exceeds the one that can be consulted and operated by an individual (Fonseca, 2006). According to this observation, the organization of the resources in online platforms presents itself as relevant, with teachers and students being able to more easily compare different materials and verify which ones fit their needs.

4.2. The use of ICT in the teaching of Chemical Equilibrium

As revised in Chapter 3, Chemical Equilibrium is one of the themes that easily propitiates the development of alternative conceptions, and the most diverse learning difficulties in Chemical Equilibrium are reported over the decades (Azizoğlu et al., 2006; Bergquist & Heikkinen, 1990; Cheung, 2009; Furió et al., 2000; Hackling & Garnett, 1985; Huddle, 1998; Solaz & Quílez, 2001; Tyson et al., 1999; Van Driel et al., 1999; Van Driel & Gräber, 2002).

Several suggestions have been presented through the years in order to avoid the difficulties such as: use of research conclusions to implement curriculum resources and pedagogical approaches (Pedrosa & Dias, 2000); use of correctly sequenced experiences (Van Driel et al., 1999); use of new resources apart from dialogue methods, course books and experimental activities (Huddle, 1998); help students in setting up visible images from invisible processes (Russell, 1988).

Van Driel, De Vos and Verloop (1999) proposed the use of a series of properly sequenced experiments with the aim of demonstrating the reversibility of reactions, incomplete reactions and finally the dynamic equilibrium. It is thought that the change and mixing of colors, associated with pertinent questions, is evidence of the three aspects mentioned above. Other authors suggested the use of new resources as well as methods of dialogue, manuals and experimental activities.

CE is a difficult concept to understand, given the degree of abstraction required, which appeals for the use of concrete examples. These concrete examples could be laboratory experiments carried out in class. However, although these are of great importance for understanding the events associated with chemical equilibrium at the macroscopic level, they continue to imply an extra abstraction layer to understand what is happening at the microscopic level. This condition is related to the model of Chemical Equilibrium and constitutes one of the factors that favors the use of simulations: the reduced scale of the molecular level. Thus, to reach the concrete examples mentioned above, the solution may be the use of analogies and simulations (Huddle et al., 2000; Russell, 1988; Wilson, 1998).

The analogy corresponds to the use of a relation of similarity between the actual concept and a given situation. When they have the pretension to represent a system or a process, by a model, as if it was that system or process, they constitute simulations. In turn, if these simulations are supported by the computer, they become computational simulations.

An important feature of the simulations and analogies is the attempt to turn the concept of Chemical Equilibrium more accessible and understandable to students, either by a dynamic model or by comparison with everyday situations (Van Driel & Gräber, 2002). The analogies that allow the understanding of the concept are seen as a possible constructivist strategy (Duit, 1991 quoted by Huddle et al., 2000).

Thus, some digital resources are considered particularly relevant in the teaching of formal or complex concepts, because of their ability in representing abstract models as in the case of simulations (Mintzes et al., 1998, Russell et al., 1997, Sarıçayır et al., 2006, Sprague et al., 2005); computers enable the microscopic and macroscopic representation of a certain phenomenon at the same time (Russell et al., 1997). We found here a basis for the use of simulations when we intend to facilitate abstraction, necessary to understand certain phenomena, as in Chemical Equilibrium that is associated to a microscopic model. In the concrete case of teaching Chemical Equilibrium, references point out the relevance of the ICT use (Hameed et al., 1993; Huddle et al., 2000; Karpudewan et al., 2015; Paiva et al., 2002; Russell et al., 1997, Sandberg & Bellamy, 2003, Sarıçayır et al., 2006, Sprague et al., 2005) recommending, in particular, the use of computer simulations.

Pedrosa and Dias (2000) referred that the use of the conclusions from the investigations are essential for the improvement of the teaching of chemistry. Banerjee (1991b) suggested several decades ago that one of the reasons why there is apparently no good use of research on CE teaching is related to the absence of modules for its teaching, ready for use by teachers and elaborated considering misconceptions and conceptual difficulties diagnosed in the students. As seen in the previous section, more recent references continue to notice that websites sharing scientific content and resources should be more careful in adapting to the curriculum and teachers' needs (Weigold & Treise, 2004). Also, Van Driel and Gräber (2002) point out that although several authors defend a thermodynamic approach to Chemical Equilibrium, based on scientific convictions and criticism of kinetic approaches and formulations of the Le Chatelier principle, there are no modules based on thermodynamics for teaching though it would be interesting to verify in practice its efficiency and feasibility.

It is interesting to notice that different references have presented, while the capabilities of computers were less widespread, strategies based on physical analogies and simulations.

Huddle, White and Rogers (2000) aiming the constructive integration of concepts, presented simulations in the form of games in which students participated physically, as an analogy to the microscopic events that lead to the establishment, maintenance, disturbance and reestablishment of Chemical Equilibrium.

To introduce the analogy it is provided to the students a box with cards, colored on one side and white on the other. Next, pupils are given fractions of colored and white cards with enough energy to change color. Working in pairs, students are running cycles, where one takes care of turning the colored cards and the other the white cards. After each cycle, the number of colored and white cards present is recorded, as well as the number of cards of each color that have been exchanged. In one of the games, the Le Chatelier principle is illustrated by the addition of a given number of cards to the established equilibrium, with the students having to perform new cycles and verify the restoration of balance. Starting with colored or white faces and regardless of the fractions of cards that change color, it is verified that in all games a state is reached in which the number of cards of each color stays constant throughout the cycles, as well as the number of cards exchanged per cycle.

By requiring students to identify similarities between the analogy and Chemical Equilibrium, colored cards are associated with reagents and white cards with products, concentrations are determined with the volume of the box. In this way, graphs of the concentration over time are obtained similar to those of actual reactions. Students calculate the equilibrium constant and relate the achievement of values greater or less than one with the fact that the fraction of reactants with energy to become products is higher or lower than the fraction of products with energy to transform into reagents.

The number of cartons of each color turned per cycle is associated with the rate of the forward and reverse reaction, allowing to conclude that the rate of the forward reaction decreases and the rate of the inverse reaction increases until the equilibrium is reached, where they equalize.

In what concerns to the principle of Le Chatelier, students could understand through the game that the addition of more reagents does not change the equilibrium constant.

The authors note that students should be informed that the major limitations of the analogy relate to the fact that the cards are two-dimensional and that collisions are not a requirement for the “reaction” to take place.

This work (Huddle et al, 2000) inspired the group in the creation of a computational simulation for the teaching of Chemical Equilibrium in a previous project - master degree (Fonseca, 2006). The following table illustrates how the analogy from Huddle, White and Rogers (2000) contradicts common alternative conceptions in this theme.

Table 4-1 Misconceptions and the use of an analogy.

Misconception	Relation to the analogy
The rate of the forward reaction increases from the start of the reaction to equilibrium.	The data collected illustrates that the rate of direct reaction always decreases until equilibrium is established.
The reverse reaction only begins to occur after the forward reaction is complete.	During the games the direct and reverse reactions are simultaneously occurring.
At equilibrium, the concentration of products is always equal to the concentration of reactants.	In none of the games are the equilibrium concentrations of the reactants and products the same.
The addition of a reagent to the system in equilibrium, alters the equilibrium constant.	By adding regents, the reaction continued to occur in both directions. The equilibrium was reestablished, maintaining the equilibrium constant.
When a reagent is added to the system, there is a drastic change in the balance.	After reagents are added to the system and the equilibrium is restored, the amount of reagents is higher than that which existed before addition to the system was imposed.

The simulations were tested in several audiences, with appreciable improvements in students who already have some knowledge about CE. However, as might be expected, these benefits are not significant for students who do not have knowledge about this topic.

Wilson (1998) proposed a teaching-learning activity very similar to the exchange of cards described above, which has proved to be efficient in many countries over the years.

Sawyer and Martens (1992) proposed an equilibrium machine to reproduce in a practical way the establishment of the equilibrium state after a certain time of conversion of reagents into products and products into reagents. It operates through an air pressure tube that moves balls (placed in compartments) that have to rise to a certain altitude in order to pass the activation energy barrier (materialized by means of a vertical board of a certain height placed between the compartments).

One of the most important challenges for the chemistry teacher is helping students to form visible images of invisible processes (Russell, 1988). This author reports in his article several types of common analogies used in the teaching of Chemical Equilibrium. Among them, we mention the case of the liquid transfer model: there is passage of liquid between two tubes until a state is reached in which the volume of liquid transferred from A to B is equal to that transferred from B to A and thus, the system reaches equilibrium. In this model, the analogy is similar to the use of cards.

As already mentioned, other authors suggest computational simulations rather than physical experiments to establish analogies with Chemical Equilibrium. Hameed, Hackling and Garnett (1993) propose a computer-aided instruction package as a way to enable conceptual change in students. This package also includes simulations, through the use of dynamic graphics. It was concluded that the modules were more successful in cases where conceptual change was followed closely, generating a cognitive conflict with the students' previous ideas. Through computer-generated dynamic graphs, simulations can facilitate the learning of abstract concepts (Bragin, 1996).

The use of a program involving simulations and simultaneous visualization of macroscopic and microscopic events, developed by Russel, Kosma, Jones, Wykoff, Marx and Davis (1997) demonstrated an increase in the understanding of the characteristics of Chemical Equilibrium and the decrease in the use of misconceptions on the part of the students.

Huddle, White and Rogers (2000) reported the passage of the card simulation described, initially physically made, to the computer. They emphasize the variety of options that the computer makes possible against physical simulation, but warn that computer application results are more effective if students play it first physically.

In fact, to overcome the conceptual difficulties of students with the dynamic model of CE, several digital resources have been developed, involving the use of computer activities to help students make mental constructions, with results that are encouraging (Dubinsky, 2002).

Articles continue to point it is necessary for high school chemistry teachers to make greater use of alternative instructional strategies like computer simulations (Kahn, 2011). Simulation technology appears to afford teachers and students with the capacity to: compile information between variables in order to generate relationships, provide an environment to make comparisons between data and visually draw attention to patterns and contrasts using graphs and animations. Students are also able to test assumptions, dynamically regenerate graphs, and view graphics at the molecular level with computer simulations. Students report that simulations helped them to critically analyze a problem, make unobservable processes more explicit, and contribute to their science learning in ways that go beyond textbooks (Kahn, 2011).

There is no certainty that the use of computer simulations will necessarily benefit all students. In a study conducted in the US, students with lower prior knowledge of chemistry concepts were more likely to use computer simulations to confirm their predictions about particular concepts than students with higher prior knowledge (Liu et al., 2008).

The selection of the most appropriate material is one of the challenges, in the diversity of digital resources available online for the teaching of CE. Thus, while on the one hand this allows learning materials to be found more easily, on the other hand it causes some difficulty in the selection and organization of knowledge construction. The strategy for applying the simulations is another of the factors with possible implications for success. All simulations and analogies have in addition to similarities, differences within the concept. These differences, if not immediately identified and explained, could destroy the purpose of using a simulation, leading to new misconceptions (Harrison and Treagust, 1994 cited by Huddle et al., 2000). According to the theory of alternative conceptions, the teacher should begin by questioning the students about the subjects in order to discover the wrong ideas they have. Next, you should adopt methodologies that demonstrate to students the failure of their conceptions. If these methodologies are concerned with the use of a simulation, it is important to point out the differences between the model and the actual concept.

Recent studies suggest that ICT can be more effective if accompanied by orientation strategies (Sarıçayır et al., 2006). “The study shows that computer animations might prove to be an invaluable means in the teaching of dynamic equilibrium. The animations used in this study, unlike those in similar ones, employ the presentation of dynamic equilibrium at molecular level, thus helping increase students’ awareness of the subject and hinder formation of misconceptions” (Sarıçayır et al., 2006).

Exploration guides for exploring a particular application (Paiva & Costa, 2010), encompass several tasks, such as answering questions, recording data and reflections. The exploration guides may be useful to counteract some dispersion of the students in the process of using ICT (Paiva & Costa, 2010). Concerning the "Le Chat" program (Paiva et al., 2002), the students who used them presented better results than those who did not use them. WebQuests appear as another example of a strategy for the application of ICT in education, constituting oriented research activities, where part or all of the information that the students interact with comes from resources available on the Internet (Dodge, 1997).

Summing up, several publications show the importance of using ICT in the teaching Chemical Equilibrium. In fact, a considerable amount of resources are available online for teaching this theme, nevertheless we continue to see reports of difficulties and misconceptions. “Despite a body of literature on the use of computer simulations in science classrooms, comparatively little research has been done on how to teach with this technology” (Khan, 2011). This scenario should stress the importance of carefully planning the design and use of ICT approaches, taking under consideration points like the conclusions from previous studies, the relevance of the materials involved and the role of the teacher.

Chapter 5 - Development of a new approach, based on the use of digital resources, to promote facilitated abstraction in Chemical Equilibrium learning

5.1. Facilitated Abstraction – an idea that emerged throughout the project

“Anyone who has ever tried to present a rather abstract
scientific subject in a popular manner
knows the great difficulties of such an attempt.”
Albert Einstein (1879-1955)
In Lincoln Barnett *The Universe and Dr. Einstein,*
William Sloane Associates, New York, USA, 1948

Chemical Equilibrium is a subject saturated with digital resources, but studies in the field still refer the lack of well-planned educational modules based on ICT and the prevalence of the same learning difficulties reported decades ago (Cheung, 2009; Erdemir et al., 2000; Furió et al., 2000; Solaz & Quílez, 2001; Van Driel & Gräber, 2002). By the time this project was purposed and initiated, the central goal was to investigate how to take advantage from ICT potential in the teaching of Chemical Equilibrium. The main innovation of the project was predicted to reside in:

- the design of an educational approach for the teaching of Chemical Equilibrium based on the findings and directives from literature, both concerning Chemical Equilibrium teaching and the use of ICT in education;

- the conduction of a case study to investigate how this theoretically grounded approach works out in classroom environment.

The notion of "facilitating abstraction" was inspired in the literature demand for improving the learning of Chemical Equilibrium, recognized as an abstract concept, while taking advantage from ICT's potential.

The idea of "facilitating abstraction" was not a preconceived goal of this investigation, which had a more general starting point, as exposed above. Instead, it was a concept that arose during the first steps of the project.

The term[6] emerged in the phase of literature review in Chemical Equilibrium teaching, which recurrently labels chemistry as being abstract and blames that nature of this science for great part of students' difficulties and misconceptions. On the other side, studies on ICT reveal their educational potential in abstract subjects. So, "facilitating abstraction" appears to be one of the major demands to improve the learning of Chemical Equilibrium and at the same time one of the ways to potentiate ICT use in education. Following this reasoning, the concept started growing in importance along the way, leading to a shift in attention that narrowed the goal, but, at the same time, clarified the road of the project. The main goal can be rephrased to: how to get advantage from ICT's potential in order to facilitate abstraction in the learning of Chemical Equilibrium. The innovation vertices referred above didn't suffer from this specification, instead a new source of innovation rose:

- conceive and apply an approach specifically designed for facilitating abstraction in the learning of Chemical Equilibrium.

The sense in which we interiorized the meaning of the word abstraction (and consequently its facilitation) was the one implicit in chemistry education literature. This meaning will be later discussed in this chapter, and was one of the targets in the state of art review, influencing our educational approach design. Nevertheless, along with the development of the project we felt some theoretical need of clarifying and situating our use of the word abstraction in the big picture of its meaning, which led us to call upon the

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[6] On the literature we find the theoretical framework "reducing abstraction" especially in the field of mathematics learning. Nevertheless this concept is centered in a self-process of reducing abstraction entirely promoted and conducted by the student alone (Hazzan, 1999). Our purpose is to aid the student with exterior actions in order to help him achieve the necessary level of abstraction to understand concepts.

philosophy of science and cognitive psychology. Several publications focus on studying the importance of considering the reasoning students learn by in order to design effective teaching strategies (Dubinsky, 2002; Wu et al., 2003). The fundamental lines of this review, presented below, will be crossed, in later chapters, with the content of the approach designed and the results from the case study. From this approach, we intend to frame our work while considering the broader multidisciplinary concept of "abstraction", and shine a light over promising investing avenues for further investigation.

5.2. Review about the "abstraction" concept

> *"There is . . . a rhythm and a pattern between the phenomena of nature which is not apparent to the eye, but only to the eye of analysis; and it is these rhythms and patterns which we call Physical Laws…"*
>
> **Richard Feynman** (1918-1988)
> In *The Character of Physical Law*

The term "abstraction" results from the translation of the Greek word "αφαιρεσις", meaning "detachment", to the Latin "abstractio*"* made by Boethius (Universal Encyclopedia of Philosophy). The original literal meaning consists in taking away something from an object (Bäck, 2014). The distinction between concrete and abstract entities emerged as early as the time of Plato (in his theory of forms) to separate the imperfect realm of sensation from the perfect realm of forms (Christoff & Keramatian, 2007), giving these an independent, substantial existence (Bäck, 2014). Thomas Aquinas, also defends that in formal abstraction *both items remain*, Aquinas' doctrine may be read as saying that to do abstraction is to "hide" some of the true sentences while keeping other true sentences visible (Angelelli, 2004). Aristotle replaced this idea for a more interactive perspective between concrete and abstract concepts, referring that abstract entities do not have a separated existence but only exist in the concrete objects or events they are abstracted from, "they are real although not independently real" (Bäck, 2014). Hicks explains Aristotle's perspective in the context of mathematical objects: "they are obtained by abstraction from things of sense, by whose existence their very existence is conditioned" (Hicks, 1907). According to Aristotle higher-order knowledge consists in generalizations, summaries of recurring features of experience (Ohlsson & Lehtinen, 1997). Aristotle's view reflects the classical doctrine of abstraction, defining this concept as the general representation of all the particular situations of a certain kind, giving us the essence of the kind (Radder, 2006). Abstraction is a procedure that gives general concepts by comparing particular situations, leaving out the irrelevant and mentally setting apart what is relevant and common (Radder, 2006). In other words it is an operation of intellect by which objects of knowledge are separable from their matter (Hicks, 1907). Abstraction presupposes experience but is not based on a complete enumeration of cases. Moreover, in some cases, one or a few cases suffice to abstract the universal, but they have to pass the test of verification (Crespo, 2009).

In present days "abstraction" is defined in a regular dictionary or encyclopedia by sentences like:

- the quality of dealing with ideas rather than events (Oxford dictionary online);
- the cognitive process of isolating a common feature or relationship observed in a number of things, or the product of such a process[7]. (Encyclopedia Britannica online);
- operation of the intellect consisting in detaching and retaining some property of a thing as a basis to form a cognitive image or a concept (an abstraction) of that thing (Polish encyclopedia of philosophy).
- it is the opposite of specification, which is the analysis or breaking-down of a general idea or abstraction into concrete facts (Wikipedia).

On the literature about abstraction and abstract reasoning[8] similar general definitions can be found:

- The capability of thinking about ideas that are removed from the facts of the "here and now" and from specific examples of the things or concepts being thought (Ylvisaker, 2006).
- It is what the mind is able to form when stimulated in the absence of a concrete subject (Snead, 2011).
- Every day (English) language retrieves three possible meanings. One is 'leaving out' (from the conceptual interpretation the original process everything but its result), one is 'setting apart' (the conceptual result of an observational process is separated from the original process), and one is 'summarising' (implication that

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[7] Abstraction can both mean the act of abstract or to the state of being abstracted (Radder, 2006) "Abstraction", in this document will be mainly used to refer to the process. The term "abstract concept" is an alternative that we will adopt to mean the product of abstraction.

[8] In literature the expression "Abstract reasoning" is also common; sometimes used to refer to the "act of abstracting" but also as "reasoning with abstract concepts", as the ability on the basis of a generating concepts but also the capability of using those concepts for different purposes and in difference mental operations.

two particular situations are observed non-conceptually, so as to abstract what is common and general about them) (Radder, 2006).

"Abstraction" is typically defined as the mental process of formulating general concepts by retaining only the relevant properties for such purpose. Abstraction allows detaching from concrete objects and/or events, dealing instead with ideas.

Recapping the story so far, "abstraction" is usually referred as the mental process of formulating general ideas or concepts by detaching from concrete objects and/or events and retaining only the relevant properties for such purpose. In this "typical" definition the meaning of abstraction in contemporary sources stays close to the one theorized by Aristotle. Nevertheless, in the field of philosophy (of Science) and psychology a lot has been written about the process and the product of abstraction. There are several attempts of finding a deep meaning for abstraction in the literature, giving rise to different perspectives. This diversity confers some ambiguity to the word (Christoff & Keramatian, 2007) and turns difficult the task of elaborating a detailed definition of abstraction: abstraction has several meanings both in everyday language and philosophy (Radder, 2006); "there is a lack of intrinsic form in the term, sometimes it is just left undefined" (Christoff & Keramatian, 2007); Different kinds of abstraction are associated with different cognitive resources and the relevance of them vary according to contextual factors (Martínez & Huang, 2011). Philosophers have developed several conceptions of abstraction which reflect theirs philosophical positions (Bäck, 2014). It has never been clear how the process of abstraction is supposed to work. Despite a consensus on the *importance* of idealization and abstraction, there is not much consensus on what these things *are*, and what exactly they achieve (Godfrey-Smith, 2009).

There are multiple references pointing the ambiguous meaning of "abstraction" when it comes to a more detailed definition of the concept.

In this project we do not intend to perform an exhaustive review about the process of abstraction in literature, since Psychology and Philosophy of Science are not the central subjects of this thesis, nor the expertise area of the group. For the same reasons, we intend even less to take party for one of the views about the nature of abstractions. Nevertheless, for our purpose of facilitating abstraction in the learning of Chemical Equilibrium it is important to clarify the meaning and the scope of “abstraction” in Chemistry Education, which is rarely stated and very often taken for granted in literature on the field. So, we follow several authors who defend that a plurality of abstraction practices is relevant (Martínez & Huang, 2011), reviewing next some perspectives in order to be conscious of the multiplicity of interpretations surrounding “abstraction”. Crossing those views with publications about Education in Chemistry, we intend to better understand the meaning carried by this word in this field.

After **Plato** and **Aristotle,** already referred accounts on abstraction, other thinkers have tried to delve in the matter, transposing the discussion from external entities to processes inside the mind (Christoff & Keramatian, 2007). Aristotle holds the things abstracted to reflect reality, instead later philosophers, as Jonh Locke and Berkeley, sustain that we make general concepts for our convenience (Bäck, 2014). Aristotle didn’t view the process as psychological or epistemological (Bäck, 2014). **Locke** featured abstraction as a mental process from which more general ideas are obtained by isolating individual qualities from particular beings, becoming general representatives of all of the same kind. General ideas are free from space and time constraints (Christoff & Keramatian, 2007). In Locke’s words *“Abstraction”* involves an operation by which something is *retained* and something else is *left out* (Locke. 1959 cited by Angelelli, 2004). Locke, the philosopher perhaps most strongly associated with the idea that universals are derived by abstraction from empirical data (Thorntom, 2003).

Locke focuses in describing abstraction as a mental concept but the definition is still close to that of the classical doctrine. Abstraction is still very much linked to the formation of general ideas by summarizing commonalities from experience. More than a century later, **Bertrand Russel** still treats abstraction as being close to generalization (Laurence & Margolis, 2012), so this was a meaning that prevailed in History. Some authors like Angelelli (2004) defend that we should have never left this definition: “This genuine meaning has been lost in the mainstream of the logical and analytic tradition of the 20th century and, what is worse, has been replaced by pseudo-uses (Angelelli, 2004).

Berkeley and Hume were critics of Locke (Laurence & Margolis, 2012). **Berkeley** counterpoised the idea of isolating qualities, referring they are present globally but when performing the abstraction there is a shift in attention[9] according to the purpose, abstraction occurs by focusing attention in a particular feature. Today this idea is still valued and referred as selective attention (Christoff & Keramatian, 2007).

David Hume seems to agree with Berkeley (Bradshaw, 1988). Also, according to Hume, things abstracted may have use for us but need not to reflect the structures of reality (Bäck, 2014). This discussion is also frequent in Epistemology of Science, known as the divergence between realistic or antirealist positions. The question can be posed, using Richard Feynman quotation in the beginning of this chapter:

> Does the scientific models about the rhythms and phenomenon of nature that go behind appearance, reflect reality or just explain it?

This discussion assumes particular relevance in chemistry, where great part of subjects involve the microscopic world, generating intangible concepts, turning then an easy target to question their true resemblance to reality. This is also relevant to understand the nature of the product of abstraction.

Besides these views, more related to philosophy of science, also on the field of psychology there have been attempts to understand abstraction and the features it involves.

Jean Piaget postulated that there are four stages of cognitive growth: sensory-motor intelligence (from birth to age two), preoperational thought (from age two until eight), concrete-operations (from age eight to twelve) and formal reasoning (Inhelder and Piaget, 1958). The most critical event is considered the transition from the "concrete" to the "formal" stage, in which logical operations such as hypothetical-deductive, combinatorial, probabilistic, and reasoning operations become available. In this context, the role of the teacher is to assure the adequacy of the learning task (Mintzes et al., 1998), while also guiding the student in his course from concrete to abstraction. **Piaget** distinguishes empiric abstraction from reflective abstraction, being the second an abstraction about concepts and actions (Martínez & Huang, 2011). Reflective abstraction is constructive and results in “new syntheses in midst of which particular laws acquire new meaning” (Dubinsky, 2002). Dubinsky (2002) refers to how Piaget's reflective abstraction is linked to the mathematical one by the fact that it is centred in the subject and in the actions that he does and not so

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[9] Bäck points that the idea of shift in attention was already present in Aristolte’s view (Bäck, 2014).

much in the properties of the objects. According to Piaget many secondary students could not have reached yet the capability of understanding abstract concepts without concrete basis (Snead, 2011). Piaget labelled the final stage of intellectual growth from concrete to abstract thinking the “formal operational stage” (Inhelder & Piaget, 1958). It is believed that only two-thirds of adults ever reach this state of abstract thinking. Moreover, this formal operational thought, or the ability to generate creative solutions for abstract issues, may not appear until age twenty or thirty (Healy, 2004).

Lakoff and Johnson propose a hierarchic system for abstraction, where abstract concepts are understood trough metaphors. In the first level there are the concrete concepts which can be understood by simple interaction in the sensorial world. Then, in the second level, there are more abstract concepts obtained from abstracting from the first ones. In the third level there are concepts highly abstract, which can only be understood by the establishment of metaphors with the concepts in lower levels. The way metaphors are selected is related to the selective attention referred by Berkeley (Christoff & Keramatian, 2007, Lakoff & Johnson, 1980).

Barsalou questions if metaphors are sufficient to form the high abstract concepts and instead purposes that concepts take the form of simulators. The fact that several simulations determine an abstract concept makes abstraction dynamic. Barsalou proposes different types of abstractions where we can see similarities with ideas form philosophy of science. Barsalou takes a pluralistic view of abstraction (Martínez & Huang, 2011).

From **Radder**’s perspective abstraction is involved not only on the operations of “setting apart” and “leaving out” but is it also in the extensibility of concepts. The author clarifies this notion as: “I call a concept extensible if it has been successfully applied to a certain domain and if it might be used in one or more new domains. (…) The sensible attempt to enlarge the scope of a concept by applying it to a materially different domain, including its novel relevance and irrelevance conditions, involves abstracting from the original realization context.” (Radder, 2006). The extensibility of the concepts turns them “non locals”, transcending the meaning they have as interpretation of the observational process made so far (Martínez & Huang, 2011). But the process by which concepts extend toward the results of new observation processes is not something fixed in principle (not necessarily also in practice) (Rol, 2007). According to Radder there is a set of conditions that could extend the concept to a new domain (Martínez & Huang, 2011). By means of abstraction the concept can be continuously restructured to include application in new domains. “For Radder there is no unique right conceptualization; at most, there is a limited set of conceptualizations suitable, even available, for our contingent purposes as cognizant humans” (Rol, 2007). This perspective differs from old doctrine view of the concepts with fixed extension, being abstracted from the world through non conceptual abstraction. Radder (2006) criticizes the old doctrine belief that non-conceptual observation is the starting point for an abstraction (Martínez & Huang, 2011), based on the typically Kantian understanding that it is impossible to know the world in the absence of structuring concepts (Rol, 2007). “In Aristotelian epistemological view, abstraction as summarizing the relevant and common aspect of different observation processes does not suffer from the problem of the prior conceptual structuring labor that our concepts do for us” (Rol, 2007). The idea of abstraction as summarizing common properties to set a kind is considered implausible by Radder. Instead, Radder believes that concepts both structure the world and abstract from it (Radder, 2006). As structuring elements concepts create a phenomenal world and as abstracting from a given world, concepts are ‘nonlocals’ (Rol, 2007). Radder also distinguishes abstraction from idealization (another common discussion in literature), attributing to the late a closer meaning to approximation than with leaving out and setting apart (Radder, 2006).

Ohlsson and **Lehtinen** (1997) states that the history of science and mathematics shows that generality is not achieved by extracting similarities from particulars, instead objects and events are seen as similar to the extent that they fit the same abstraction and that abstractions are constructed by assembling available ideas into new structures. The function of abstraction is not to provide generality but to facilitate the assembly process and to provide a different categorization of the world than the one suggested by perceptual similarities. In the classical view, similarity is an epistemologically primitive category. The similarities between two particulars are the basis for creating a generalization. In contrast, these authors suggest is that people experience particulars as similar precisely to the extent that, and because, those particulars are recognized as instances of the same abstraction. Abstraction engenders similarity rather than vice versa. (Ohlsson & Lehtinen, 1997).

The assembly hypothesis, on the other hand, separates the property of being abstract from the process of abstracting. The latter does not move from the concrete to the abstract because it operates on ideas that are abstract to begin with. The movement is across levels of complexity, not levels of abstraction or generality. **Ohlsson** and **Lehtinen** reject non conceptual observation and says that deep ideas are difficult in great part because of having other ideas as parts. New ideas are created by assembling previously acquired ideas into new structures. The result of the assembly process is a new knowledge structure that is more complex than the component knowledge structures. If the components are abstract, so is their combination. Abstractions arise by constructive processes operating on existing abstractions, not by operations on concrete experiences.

So, we can find here some resemblance between **Ohlsson** and **Lehtinen** ideas and the reflective abstraction of Piaget. "Consider the idea of dynamic equilibrium, for example, abstractly, dynamic equilibrium is a state in which multiple, parallel changes on one level of description compensate each other in such a way that the relevant system appears stable or stationary at a higher level of description. The prototypical example is a lake where inflow and outflow match each other exactly. At the molecular level, the lake is continuously changing, but because the molecules lost in the outflow are replaced by the inflow, there is no change in the water level and the lake looks unchanging to the naked eye. As this description suggests, the idea of dynamic equilibrium consist of at least the following components: The idea of simultaneity, the idea of compensation, and the idea of distinct levels of description (…) Learning is growth, not summarization." (Ohlsson & Lehtinen, 1997). "The regrouping of the appearances on the basis of what abstractions they fit, as opposed to by what perceptual similarities they exhibit, is the main lever by which human beings pry open the secrets of nature." (Ohlsson & Lehtinen, 1997).

Cartwright's view is closer to Aristotelian perspective (Crespo, 2009) raising Radder's discordance (Rol, 2007). She argues that the relation between abstract and concrete concepts […] in science is (like) that between a general truth and a specific or local model for that truth. (…) If statements are abstract enough, they tend to render true hypotheses – true, that is, of the actual world."(Cartwright, 1989 cited by Rol, 2007). The concept of abstraction, by this author, is related to the establishment of causal relations, which involves a first step of subtraction by which general principles are enunciated going upwards from experience. But it is necessary a second step of concretization where we go downward to a series of specific conclusions (Martínez & Huang, 2011). Subtraction aims to a general statement about a causal factor leaving out other potential disturbing factors, but concretization is needed to generate relevant explanations and predictions. This second step is necessary to create conditions for the application of the general law in concrete situations (Martínez & Huang, 2011). **Cartwright** also speaks about the exportability of information (a concept close to extensibility referred by Radder): “we gather information in one set of circumstances but expect to use it in circumstances that are quite different.” (Rol, 2007). Cartwright understands scientific explanation in terms of stable causes, which she calls “capacities” or “natures” (Crespo, 2009). She also defends that many abstract concepts in physics play merely an organizing role and do not seem to represent genuine properties (Cartwright,1983).

According to **Nerssian** modelling theory the aim of abstraction is to obtain generic models that allow a unified explanation of phenomena. Abstraction is closely related with mental modelling and analogical inferences (Martínez & Huang, 2011).

Other psychologists analyze abstraction in terms of its relation to semantics and will not be developed here. The level of abstraction within taxonomy refers to a particular level of inclusiveness (Rosch, 1978).

The authors differ in the way abstraction is performed, what operations can be considered abstraction and what is the identity of the product but they all agree in the importance of this operation as a key process in cognition. Table 5.1 summarizes the review made along this section and presents our ideas about the repercussions for science education.

Table 5-1 Mental process involved in abstraction (according to literature)

Mental process involved in abstraction (according to literature)		
Process		*References*
● ➡ ○	**Formulate general concepts by retaining only the properties of an object/event that are relevant for such purpose.**	Regular Dictionaries
💭	**Deal with ideas in the absence of events (removed from the facts of the "here and now"); detachment from the sensorial world.**	Old doctrine of abstraction (philosophers such us Aristotle and John Locke)
◐	**Isolate commonalities; Summarize recurring features of experience.**	
⬌	**Establish new relationships.**	
◉	**Perform a shift in attention to a particular feature, according to the purpose.**	Berkeley
💭	**Reflective abstraction requires the abilities from the formal operational stage, which is still in development in many students. Teacher must guide the student in the process from concrete to abstraction.**	Piaget
● △ ➡ ▲	**Establish metaphors with more concrete concepts.**	Lakoff and Johnson
💭💭	**Dynamic use of several simulators to understand/apply an abstract concept.**	Barsalou
✥	**Extend/enlarge the scope of a concept by applying it in a new domain (extensibility/exportability of a concept).**	Radder
⬟	**Assemble previously acquired ideas into new structures. Abstractions arise by constructive processes operating on existing abstractions, not by operations on concrete experiences.**	Ohlsson and Lehtinen
● 💭	**Obtain generic models that allow a unified explanation of a phenomenon. Abstraction is closely related with mental modelling and analogical inferences.**	Nerss
● ⇄ ○	**Establish causal relations: the first step is subtraction by which general principles are enunciated going upwards from experience; the second step is concretization going downward to a series of specific conclusions**.	Cartwright

5.3. The concept of abstraction in Chemistry Education

"Remember that every science is based upon an abstraction.
An abstraction is taking a point of view or looking at things under a certain aspect
or from a particular angle. All sciences are differentiated by their abstraction."
Fulton J. Sheen (1953) *in* Life Is Worth Living

Not only different authors defend divergent perspectives on abstraction but also the word has several meanings according to the field in which it is applied.

In everyday life, abstraction is commonly used to mean detachment from real life or sensorial world. In computer science it is defined commonly as the representation of an entity that includes only the most significant attributes (Sebesta, 2012). In the world of programming languages, abstraction is a weapon against the complexity of programming (Sebesta, 2012); this process leads to the construction of a model of a system or object that aims to simplify the "reality" using only relevant properties according to purpose, finding some resemblance with the creation of scientific models.

Haber, a scientist in the field of Chemical Equilibrium, affirmed in 1923: "The field of scientific abstraction encompasses independent kingdoms of ideas and of experiments and within these, rulers whose fame outlasts the centuries. But they are not the only kings in science. He also is a king who guides the spirit of his contemporaries by knowledge and creative work, by teaching and research in the field of applied science, and who conquers for science provinces which have only been raided by craftsmen"[10].

Literature concerning science education, published from several decades ago until the present day, frequently connects chemistry with abstraction, in some sense and extent. Chemistry is usually referred as an abstract science, involving abstract concepts or depending on a degree of abstraction ability. Next we present instances of this type of reference, some of them already mentioned in previous chapters:

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[10] — Fritz Haber - While president of the German Chemical Society, making memorial remarks dedicated to the deceased Professor Lunge (Jan 1923). As quoted in Richard Willstätter, Arthur Stoll (ed. of the original German) and Lilli S. Hornig (trans.), From My Life: The Memoirs of Richard Willstätter (1958).

- The models' importance is transversal to all science disciplines, but they are most important in chemistry because **this subject involves many abstract and complex concepts** (Halim et al., 2013);

- Another problem is the **abstract nature** of many of the characters in chemical dramas: atoms, molecules, ions, electrons, lattices, shells, etc. are all conjectured hypotheticals for which there can be no direct evidence the learner can experience. No matter how well our molecules and electrons reflect reality (if such a notion means anything) at the nanometre and picometre scale, this is not a reality that is directly accessible to the learner. The molecules and electrons we talk about in chemistry lessons are entities that have been created by scientists and teachers, as theoretical tools to think about, and talk about, our subject (Taber, 2001).

- **Chemistry curricula commonly incorporate many abstract concepts**, which are central to further learning in both chemistry and other sciences (Taber, 2002).

- **the formal structure of chemistry is an abstraction** that does not exist in any one place (Taber, 2002).

- … **chemistry instruction occurs predominantly on the most abstract level**, the symbolic level (Gabel,1999);

- Several studies have shown that students find microscopic and symbolic representations especially difficult because these **representations are invisible and abstract** while students' thinking relies heavily on sensory information. (Gabel,1999).

- There is then a multiple barrier here: learners with limited mental working space (1), are asked to use **abstract theoretical entities** (2) at a level outside their direct experience (3), to explain apparently unrelated molar phenomena at another level; when they have limited appreciation of both the role of models (4) and the nature of explanation (5). Failures to learn chemistry should not surprise us. (Taber, 2001).

- Chemistry is considered a difficult subject because it makes use of difficult language and **seems to be abstract** (Nacheva-Skopalik & Koleva, 2012).

- Chemistry textbooks continue the practice of treating **too much abstract material at an elementary physical chemistry level** (Tsaparlis, 2001).

So, abstraction and abstract reasoning appears to play a central role in the learning of chemistry. Abstraction isn't just referred as an essential process for understanding chemistry, it is also presented as an important source of learning difficulties and misconceptions diagnosed in the field. Several other sentences, although not referring directly to abstraction, present motives/recommendations related to the mental processes involved in abstraction summarized in table 5.1:

- Students mistakenly infer that characteristics applicable to one level apply to another level. Levels confusion represents a profound challenge to learning chemistry and impedes conceptual change in the discipline (Stieff et al., 2013).

- The information processing model of learning helps to explain the barriers to learning chemistry that were identified earlier: the complex nature of chemistry concepts, the threefold representation of matter, practical work, unfamiliar materials, language, and the structure of the discipline. It would appear to be more consistent with the way people learn for students to study the familiar macroscopic world first, and then explain that world using the particulate nature of matter. In this way new concepts are anchored on the concepts of a pre-existing network in long term memory. Perhaps this approach would help eliminate some of chemistry's misconceptions. In terms of short-term memory, the limited space available suggests that the three ways of representing matter not be introduced simultaneously to novice learners. However, once they are introduced, students should be given numerous opportunities to relate the three representations so that multiple linkages are formed in long-term memory (Gabel, 1999).

- …learners accept a particle model, but are unable to recognise that molecular level explanations are only useful if they have a distinct nature compared to molar level explanations (Taber, 2001).

- Reasonable understanding of the phenomena is established when all three levels of the concept cover each other, supported by visualisation elements, in specific way in students' working memory… for a meaningful knowledge we should follow the multiple representation principle. This means that it is better to present an explanation in words and pictures than only in words. (Devetak et al., 2009).

- Models are used both to make abstractions visible and, crucially, to provide the basis for predictions about, and hence scientific explanations of, phenomena (Gilbert, 2005).

- Gabel 1993 presents justifications for algorithmic learning: chemistry teaching emphasizes the symbolic level and problem-solving at the expense of the phenomena and particle levels. Another explanation is that even though it is taught at the three levels, insufficient connections are made between the three levels and the information remains compartmentalized in the long-term memories of students. A third explanation is that even if chemistry was taught on the three levels and the relationships among the levels were emphasized, the phenomena considered were not related to the students' everyday life. (Gabel, 1993).

- Although an understanding of matter is important for many reasons, research on students' understanding of matter has repeatedly and consistently shown that students' fail to obtain a deeper understanding of the particle nature of matter (Hadenfeldt & Neumann, 2014).

- While appropriate knowledge and skills must be present in the mind of the learner, it is also important to recognise that they must be accessible (able to be retrieved in a meaningful form) at the time when new material is presented. It is also important that the new material must be presented in a manner consistent with the way the previous knowledge and skills have been laid down in the long term memory (Sirhan et al, 1999).

- Tsaparlis (1997) recommends teaching introductory chemistry through three cycles at the macro, representational and sub-micro levels.

- Bodner (1991) refers the dependence of new knowledge from previous concepts and has listed several factors that may lead to misconceptions in the minds of learners. He notes the problems of rote learning where students possess knowledge without understanding. When the teacher first introduces an idea, the learner may already possess previous experience (derived from the world around, including the media), which leads to confusion (Bodner, 1991).

- "many students can be taught abstract thinking through learning progressions using concrete and practical links. The link or model that is used should be based on helping students visualize and form conceptual image of the abstraction" (Snead, 2011).

Among the possible causes for the difficulties in Chemical Equilibrium (already exposed in chapter 3) there are also highlighted aspects related to the process of abstraction necessary to understand the concepts involved in this scientific model:

- Disregard of the specific nature of this theme and excessive simplification may lead to non-valid generalizations (Tyson et al., 1999);

- Chemical equilibrium issues are solved by using an algorithm learnt by heart using drills (Bergquist & Heikkinen, 1990);

- Teachers and students demonstrate conceptual difficulties when applying too intuitive reasoning using Le Chatelier's principle (Banerjee, 1991a);

- The difficulties in the teaching of Chemical Equilibrium are related to spontaneous reasoning, that is, associated to common sense, being called functional fixation and functional reduction. Functional reduction is the tendency to reason without considering all the possible variables that can influence the solution of a problem (Furió et al., 2000).

- A cause for difficulties is related to the conceptual change necessary to reformulate the conception of chemical reactions previously assimilated, so as to adapt the concept of Chemical Equilibrium (Huddle et al., 2000; Van Driel & Gräber, 2002);

- This concept has the potential to reorganize a great number of descriptions that were previously expressed in other terms (chemical reaction, change of state, solubility and limit of solubility, etc.) and to unify total and limited transformations often regarded in dichotomous ways (Ganaras et al., 2008);

- Chemical equilibrium is composed of abstract concepts and calls for the use of analogies (Huddle et al., 2000; Russell, 1988; Sarıçayır et al., 2006; Wilson, 1998).

- It is inspired by a dynamic representation of a chemical system with the aspects of reversibility and competition between reactions, and it does not only concern the vision of a state (the extent of reaction at equilibrium) but also the shifting of the equilibrium state (Ganaras et al., 2008).

- From this point of view, the Chemical Equilibrium concept is a central and complex concept in chemistry. It is considered as one of the most difficult topics in chemistry education from a cognitive point of view (Ganaras et al., 2008).

- Chemical equilibrium structures many basic chemistry concepts. This importance allows this topic to get a central position in the chemistry curriculum (Quílez, 2008).

- Chemical equilibrium is an abstract concept demanding the mastery of a large number of subordinate concepts (Quílez, 2008).

- Dealing with this complex concept calls for an in-depth consideration of both the prerequisites for learning it and students' previous knowledge (Solaz & Quílez, 2001).

- In introductory chemistry lessons, chemical reactions are presented as proceeding to completion, taking place in one direction. As a consequence, students face several cognitive conflicts when dealing with chemical equilibrium reactions (Quílez, 2004).

- "One of these areas is the chemical equilibrium since firstly, the concepts are seen abstract and secondly, the words from everyday language are used but with different meanings" (Erdemir et al., 2000).

- Secondary students find chemical equilibrium very difficult not only because the concepts of chemical equilibrium are abstract but also because there are problems in the selection of curriculum content (Cheung, 2009).

- “In long term memory there already exists a wealth of knowledge and experience of equilibrium, but not in the chemical sense. However, the language used for both static and dynamic equilibrium is very similar in several European languages. When the chemist presents equilibrium ideas they easily find points of attachment in Long Term Memory, but almost all are wrong, giving rise to alternative frameworks (…) Concepts form from our senses by noticing common factors and regularities and by establishing examples and non-examples” (Johnstone, 2000).

In the sentences presented along this section there are subjacent several process from Table 5.1. Also they put in evidence that, in chemistry, the use of the term abstraction is mainly linked to the fact that most of the concepts to learn imply thinking with ideas that are apart from the observable events, mainly because of the symbolic and microscopic nature of chemistry**.** Also, we have the added complication of operating on and interrelating three levels of thought: the macro and tangible, the sub micro atomic and molecular, and the representational use of symbols and mathematics.

“Most things which we encounter in the world, and on which we form many of our concepts, are macro in nature. But chemistry, to be more fully understood, has to move to the submicro situation where the behaviour of substances is interpreted in terms of the unseen and molecular and recorded in some representational language and notation. This is at once the strength of our subject as an intellectual pursuit, and the weakness of our subject when we try to teach it, or more importantly, when beginners (students) try to learn it.” (Johnstone, 2000).

As students grow in chemistry knowledge, they usually base their models on previous concepts that are already part of submicro and symbolic domains and so imply abstracting from previous abstractions. In our opinion, this kind of process represents one of the main features of learning Chemical Equilibrium.

Summarizing, different authors expose a relation between difficulties in the learning of chemistry and the processes of abstract reasoning to mobilize in order to understand the concepts. Table 5.2 highlights the relation between difficulties reported in the field of chemistry teaching (mostly in Chemical Equilibrium) and the mental processes involved in abstraction (according to the previous review we have made in the field). We consider that this table constitutes an important base for designing approaches to facilitate students' abstraction in the process of learning, since we also drew some implications for teaching strategies.

Table 5-2 Mental process involved in abstraction and implications for the teaching of CE

Mental process involved in abstraction and implications for the teaching of CE			
Process		*Relation to difficulties found in the learning of chemistry and CE*	*Implications for teaching strategies*
● ➡ ○	Formulate general concepts by retaining only the properties of an object/event that are relevant for such purpose.	Excessive simplification may lead to non-valid generalizations.	Clarify simplifications / idealizations associated to a scientific model.
💭	Deal with ideas in the absence of events (removed from the facts of the "here and now"); detachment from the sensorial world.	Applying intuitive / spontaneous reasoning, that is, associated to common sense, called functional fixation and functional reduction. Microscopic and symbolic representations are especially difficult because these representations are invisible and abstract.	Expose the failure of common sense ideas in explaining certain events, exposing the need for detachment from sensorial world. Minimize the absence of concrete experiences using representations that support the ideas.
◐○	Isolate commonalities; Summarize recurring features of experience.	Students easily find points of attachment in long term memory for the concept of equilibrium but almost all are wrong in what concerns chemical equilibrium, giving rise to alternative frameworks. Words from everyday language are used but with different meaning.	Expose linguistic and conceptual differences from everyday language.
⟺	Establish new relationships.	Issues are solved by using an algorithm since the relationships are not conceptually understood; Levels confusion represents a profound challenge to learning chemistry;	Encourage students to reflect on events and predict responses in order to expose relationships. Should be given numerous opportunities to relate the three representations so that multiple linkages are formed in long-term memory.
◉	Perform a shift in attention to a particular feature, according to the purpose.	Limited work space available suggests that the three ways of representing matter should not be introduced simultaneously to novice learners.	Promote student's active learning. Establish a sequence to approach the different levels of chemical knowledge.
💭	Reflective abstraction as a kind of abstraction from the abstraction requires the abilities from the formal operational stage, which is still in development in many students.	Submicro level involves entities that have been created by scientists and teachers, as theoretical tools to think, conjectured hypotheticals for which there can be no direct evidence the learner. To minimize difficulties students can be taught abstract thinking through learning progressions using concrete and practical links.	Teacher must guide the student in the process from concrete to abstraction.

Process		*Relation to difficulties found in the learning of chemistry and CE*	*Implications for teaching strategies*
● ➡ ▲ △	Establish metaphors with more concrete concepts.	CE is abstract and calls for the use of analogies.	Appeal to analogies in order to establish metaphors with more concrete concepts.
☁ ☁ ☁	Dynamic use of several simulators to understand/apply an abstract concept.	Reasonable understanding of the phenomena is only established when all three levels of the concept cover each other.	Provide different explanations for the same concept. Follow the multiple representation principle. Relate different levels of description of a concept (macro, micro, symbolical).
✥	Extend/enlarge the scope of a concept by applying it in a new domain (extensibility/exportability of a concept).	Conceptual change is necessary to reformulate the conception of chemical reaction initially assimilated. Limited mental working space is asked to use abstract theoretical entities at a level outside direct experience to explain apparently unrelated molar phenomena at another level.	Present the convenience/evidence for extending a concept to new domains. Study the familiar macroscopic world first, and then explain that world using the particulate nature of matter. In this way new concepts are anchored on the concepts of a pre-existing network in long term memory.
⬟	Assemble previously acquired ideas into new structures. Abstractions arise by constructive processes operating on existing abstractions, not by operations on concrete experiences.	Inspired by a dynamic representation, CE does not only concern the vision of a state but also the shifting of the equilibrium state. Chemical equilibrium is an abstract concept demanding the mastery of a large number of subordinate concepts.	Help to mobilize previous abstractions and consider them as the basis for new abstractions during the design of teaching strategies. New concepts need to be anchored on the concepts of a pre-existing network in long term memory.
● ∘ ☁	Obtain generic models that allow unified explanation of a phenomenon. Abstraction is closely related with mental modelling and analogical inferences.	Models are most important in CE because this subject involves many abstract and complex concepts. Models are used both to make abstractions visible and, crucially, to provide the basis for predictions.	Use simulations to represent/interact with models, assisting mental abstraction and analogical inferences. Expose relations between different levels of description like macro and micro scale, so that students can construct a unified explanation of the phenomenon.
● ⇄ ○	Establish causal relations: the first step is subtraction by which general principles are enunciated going upwards from experience; the second step is concretization going downward to a series of specific conclusions.	Chemistry instruction occurs predominantly on the most abstract level, the symbolic level. The phenomena considered are not related to the students' everyday life.	Importance of applying concepts in context, so that knowledge acquires real meaning. Complete a cycle beginning with detachment from events to deal with ideas, which are later used to explain those events.

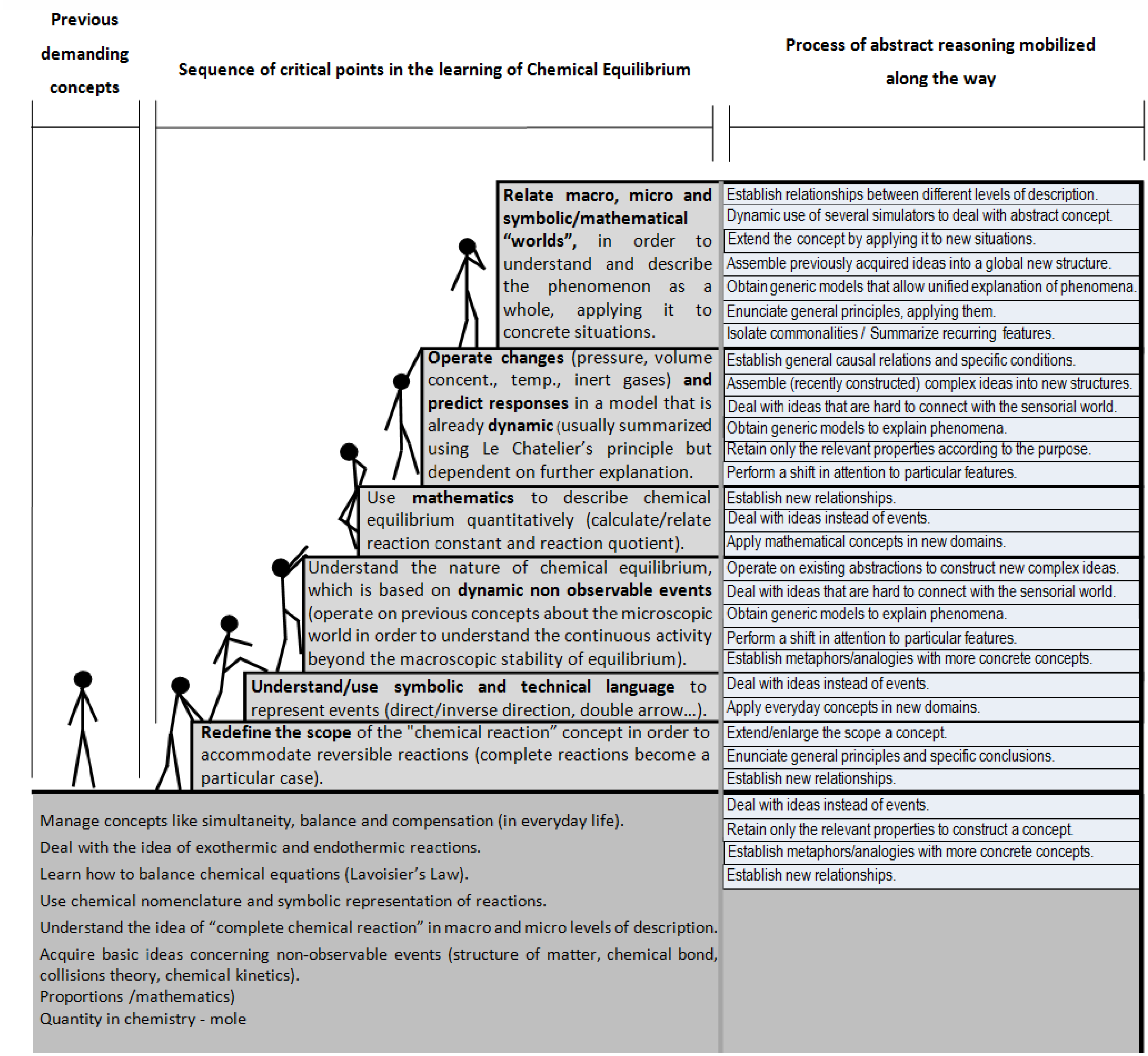
References point to the importance of teachers being aware of the reasoning developed by the students. Along the chapters of this dissertation we gathered and organized information about the reasoning that students have to carry out during the learning of the Chemical Equilibrium model. Now, we focus on the critical points for the understanding of CE highlighted by the references (the use of specific language, dealing with non-observable events, relating knowledge at three levels…) and the traditional sequence for the teaching of CE at the secondary level. We present the product of our particular reflection, metaphorically, in the form of a ladder. Our purpose is to mimic the route that the students have to accomplish when learning CE, alerting for the major difficulties and exposing the processes of abstract reasoning mobilized along the way. So, the base content of the ladder is inspired in the essential aspects reviewed in this thesis. Nevertheless, the number and the sequence of the steps as well as the height attributed to each step reflect the particular view of the PhD student according to the experience and the observations made along the project:

A) The height of each step reflects the combination of abstract reasoning processes, the mobilization of which is considered necessary to understand this particular aspect of the CE model (depth of the abstraction).

B) The sequence of the steps translates the dependence of the next knowledge on the previous concepts, the rise to a new step means to operate with the result of previous abstractions (dependency on previous abstractions).

C) The totality of the ladder (number of steps) demonstrates the multiplicity of formal processes of reasoning necessary for the whole (multiplicity of abstractions).

Observing Figure 5.1 we can notice the importance of developing teaching strategies that "support" the formal reasoning necessary for the understanding of the CE model.



5.4. Designing a new approach to facilitate abstraction in Chemical Equilibrium learning (FACE)

The concepts of Chemical Equilibrium are the result of a model used by scientists to describe this phenomenon, being constructed based on interpretations that go beyond what is directly observable, taking into account the corpuscular theory of matter and involving multiple variables. According to the bibliographical review presented in the previous sections, different authors point out difficulties in the teaching / learning of Chemical Equilibrium, providing explanations about their origin. Among the possible causes for the difficulties are highlighted aspects related to the process of abstraction necessary to understand the concepts involved in this scientific model. References also point for the pedagogical potential of computational resources when dealing with abstract concepts.

Following this trail of ideas we intend to introduce an ICT-based teaching strategy that facilitates the process of abstraction during the learning of Chemical Equilibrium. The approach we present includes the following components: a central resource (computer simulation), a support material for the simulation application (exploration guide) and auxiliary materials for the teacher (Paiva & Fonseca, 2009).

First let us focus on the central resource. The simulation we intend to use was constructed during a previous work in the field (Fonseca, 2006). This resource allows to:

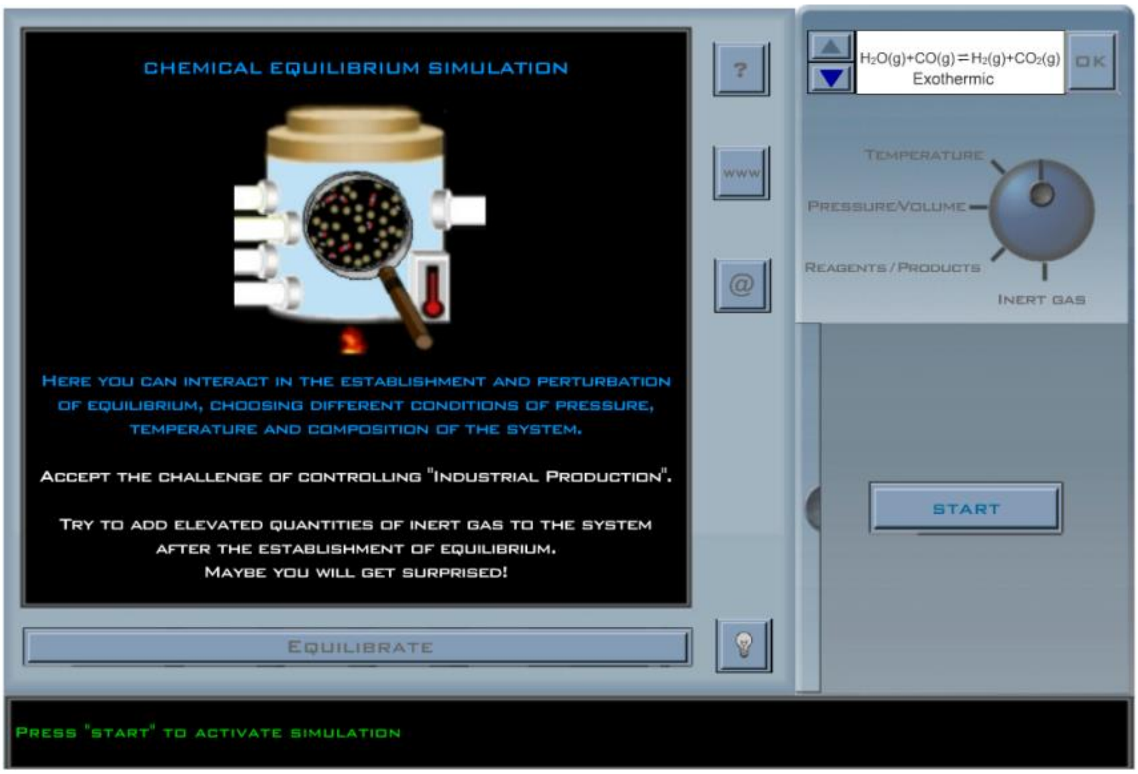
A) quantify the evolution and state of a reactional system, presenting the result of calculations in Chemical Equilibrium, starting from manipulable initial conditions;

B) provide qualitative, intuitive information on the evolution and state of the system;

C) represent the system microscopically, by means of an illustrative analogy of the variations of composition and molecular movement;

D) association with the industrial process through a symbolic analogy.

The prototype developed within the scope of the master degree dissertation is available at http://nautilus.fis.uc.pt/cec/teses/susana_fonseca/. When entering the address, after selecting the language of the built prototype(since the resource is available in Portuguese and English versions), an initial simulation presentation screen appears and the "start" button is available (Figure 5.2).



HERE YOU CAN INTERACT IN THE ESTABLISHMENT AND PERTURBATION OF EQUILIBRIUM, CHOOSING DIFFERENT CONDITIONS OF PRESSURE, TEMPERATURE AND COMPOSITION OF THE SYSTEM.

ACCEPT THE CHALLENGE OF CONTROLLING "INDUSTRIAL PRODUCTION".

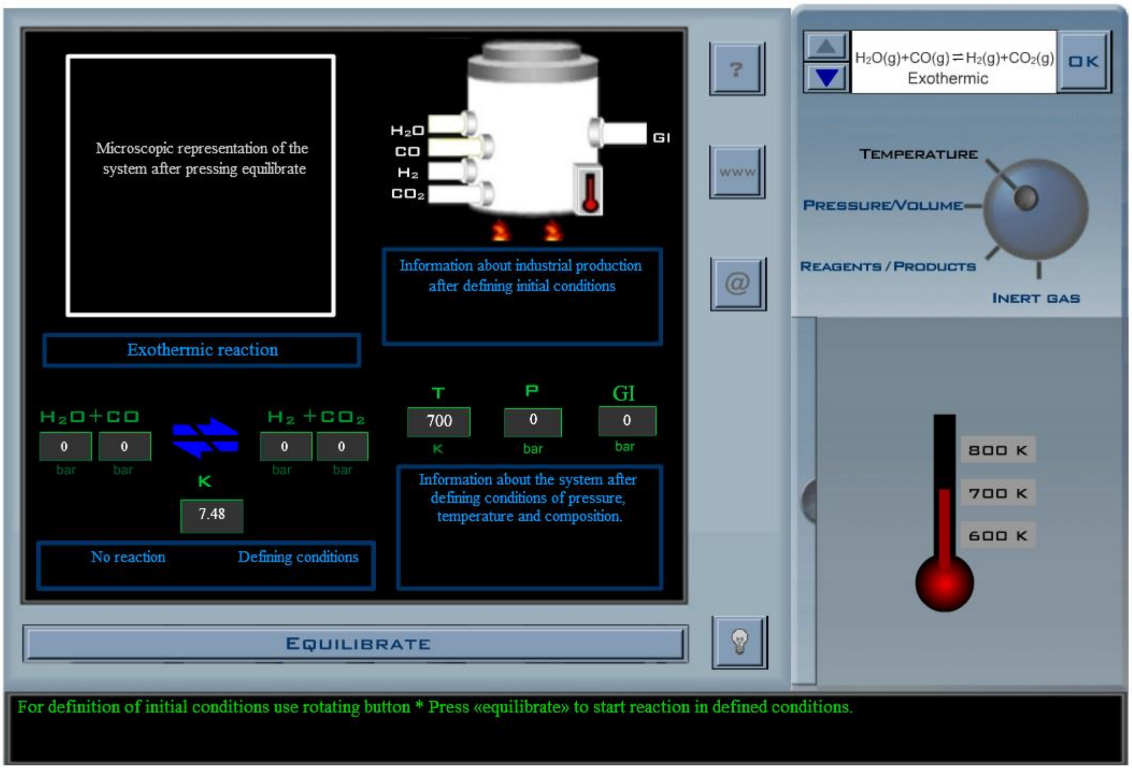
TRY TO ADD ELEVATED QUANTITIES OF INERT GAS TO THE SYSTEM AFTER THE ESTABLISHMENT OF EQUILIBRIUM. MAYBE YOU WILL GET SURPRISED!

PRESS "START" TO ACTIVATE SIMULATION

Figure 5-2 Initial presentation screen of the simulation.

After selecting the reaction (only one is available since the simulation was constructed as a prototype for further testing), the "rotary knob" becomes active and it is possible to define the initial conditions. When you press the corresponding texts for the variables, the right panel opens so that the information appears for the factor that is being configured.

For the temperature, an analogy is made with a thermometer (Figure 5.3), pressure / volume variation is illustrated with a vessel, a plunger and a barometer (Figure 5.4). For the reagents and inert gas, simple selection buttons are used (Figure 5.5). It should be noted that as the values for each of these factors are chosen, this is illustrated in the small "main-screen" reactor. The temperature is associated with more or less "flames", the volume with greater or lesser height of the reactor, and the addition of reagents / products or inert gas to the staining of the respective connecting tubes. The addition / removal of reagents and products is further enhanced by the appearance of the respective molecular models (over their position in the reaction equation).


$H_2O(g)+CO(g)=H_2(g)+CO_2(g)$ Exothermic

Microscopic representation of the system after pressing equilibrate

Information about industrial production after defining initial conditions

Exothermic reaction

$H_2O + CO$: 0 bar, 0 bar

$H_2 + CO_2$: 0 bar, 0 bar

K: 7.48

T: 700 K

P: 0 bar

GI: 0 bar

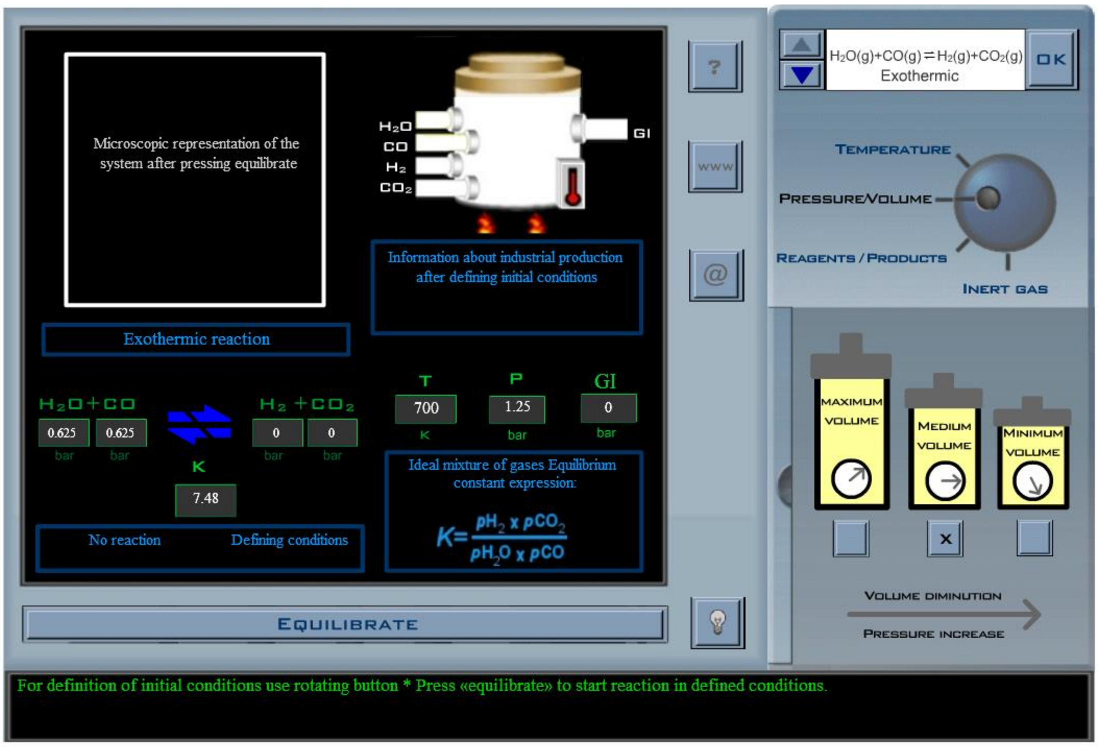
Information about the system after defining conditions of pressure, temperature and composition.

No reaction

Defining conditions

For definition of initial conditions use rotating button * Press «equilibrate» to start reaction in defined conditions.

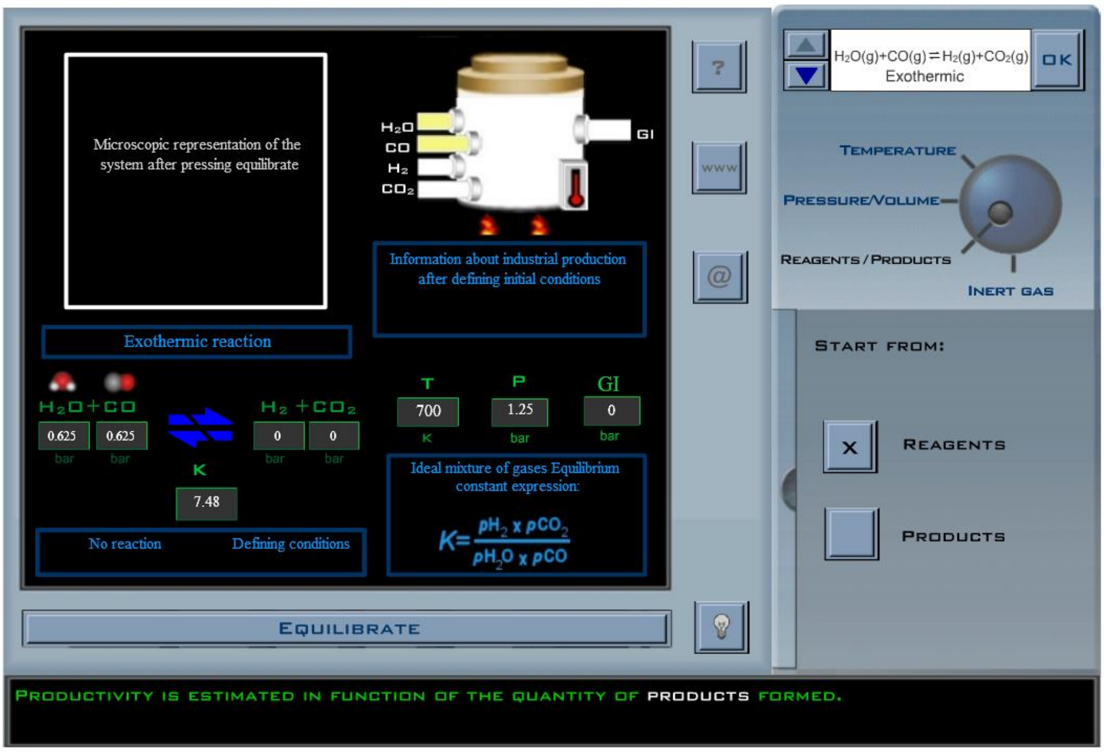
Figure 5-3 Selecting temperature.



$$K=\frac{pH_2 \times pCO_2}{pH_2O \times pCO}$$

For definition of initial conditions use rotating button * Press «equilibrate» to start reaction in defined conditions.

Figure 5-4 Selecting pressure/ volume conditions.



$$K=\frac{pH_2 \times pCO_2}{pH_2O \times pCO}$$

PRODUCTIVITY IS ESTIMATED IN FUNCTION OF THE QUANTITY OF PRODUCTS FORMED.

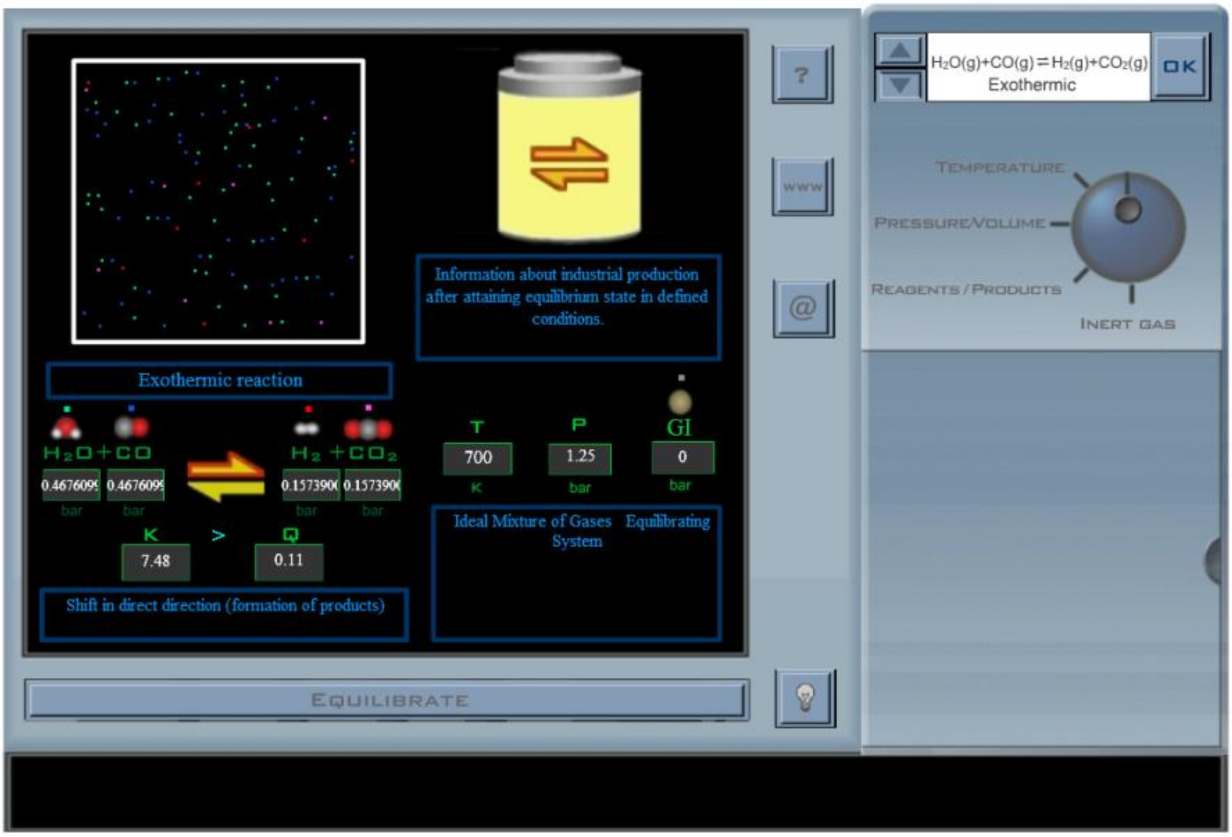
Figure 5-5 Selecting initial conditions (reagents or products).

Pressing the "equilibrate" button, the simulation displays a series of data, which is being updated continuously, to simulate the evolution of the system.

The microscopic representation changes according to a variation of the partial pressures of the reacting species. The degree and speed of movement are temperature dependent. We chose to establish an analogy between the particles of the intervening species and small colored dots in constant movement. The number of visible points of each species will be proportional to the partial pressure of the species, in this way this simulation is directly related and dependent on the model that quantifies the equilibrium.

The value of the reaction quotient (*Q*) is presented and constantly actualized until it reaches the value of equilibrium constant (*K*). There are also logical operators visible between *Q* and *K*. The indication of the direction of displacement is given via textual information and symbolic arrows, in which there is a stress marker in the direction in which the equilibrium is shifting. The reactor is presented closed and textual information is provided when the reaction is evolving to the equilibrium state.

Next, a temporal sequence of images of the simulation is presented, from the moment in which "equilibrate" is pressed until the equilibrium state is established (Figure 5.6).



$H_2O(g)+CO(g) = H_2(g)+CO_2(g)$
Exothermic

Information about industrial production after attaining equilibrium state in defined conditions.

Exothermic reaction

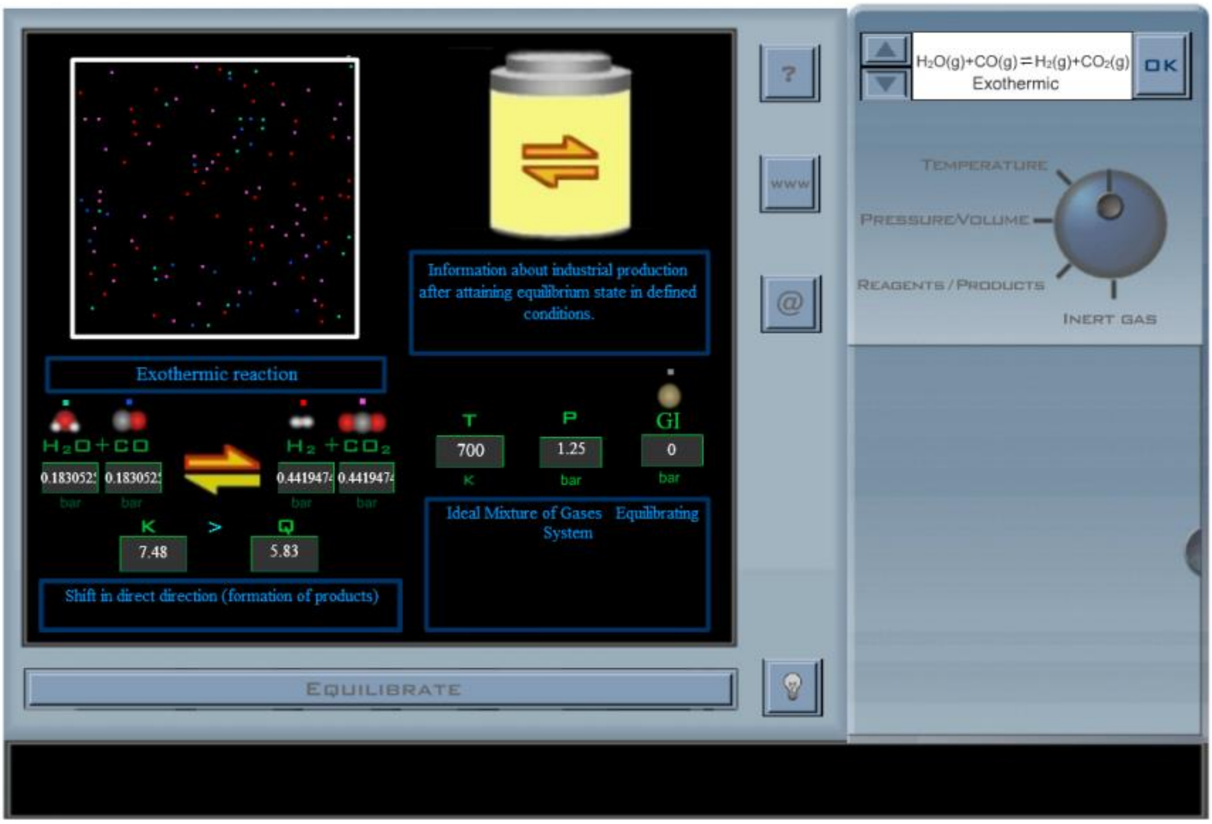
H_2O 0.467609 bar
CO 0.467609 bar
H_2 0.157390 bar
CO_2 0.157390 bar

T 700 K
P 1.25 bar
GI 0 bar

K 7.48 > Q 0.11

Shift in direct direction (formation of products)

Ideal Mixture of Gases Equilibrating System



Information about industrial production after attaining equilibrium state in defined conditions.

Exothermic reaction

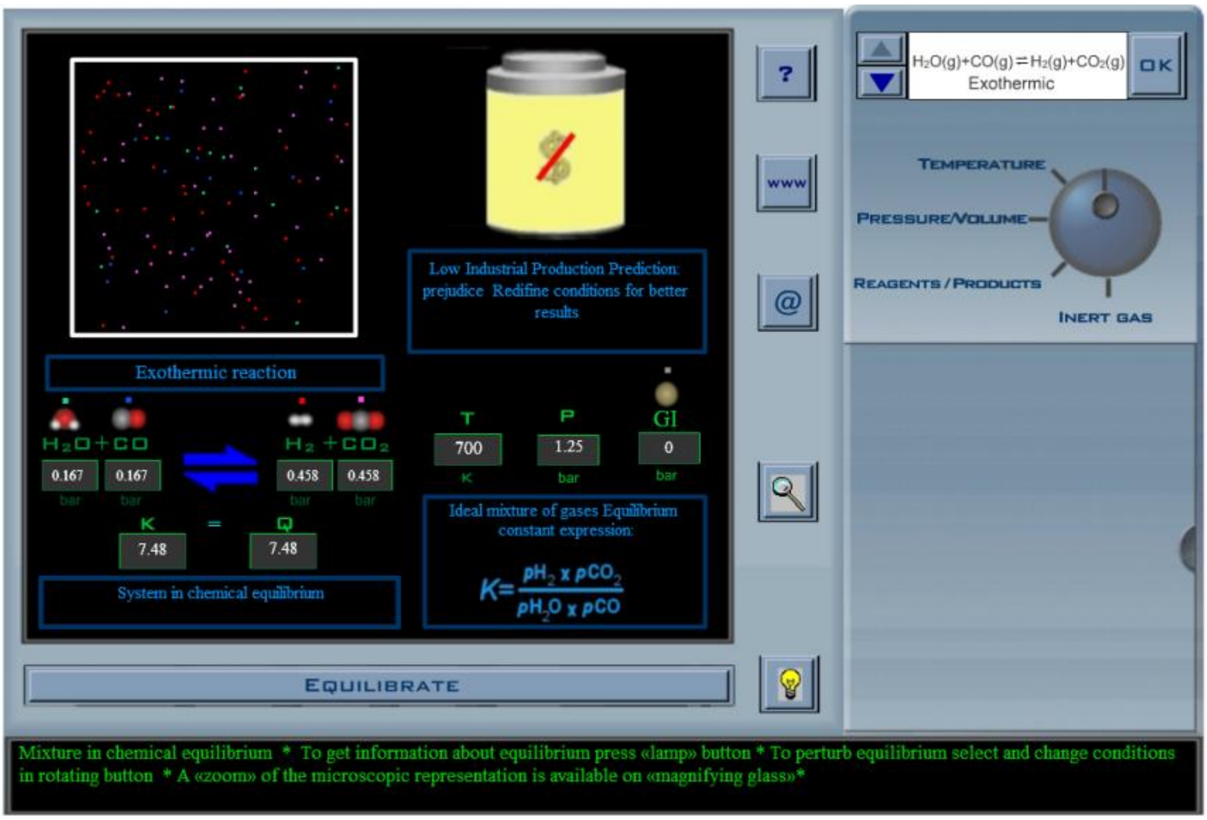
H_2O: 0.183052 bar; CO: 0.183052 bar; H_2: 0.441947 bar; CO_2: 0.441947 bar

T: 700 K; P: 1.25 bar; GI: 0 bar

K > Q: 7.48 > 5.83

Shift in direct direction (formation of products)

Ideal Mixture of Gases Equilibrating System



Low Industrial Production Prediction: prejudice Redifine conditions for better results

Exothermic reaction

H_2O: 0.167 bar; CO: 0.167 bar; H_2: 0.458 bar; CO_2: 0.458 bar

T: 700 K; P: 1.25 bar; GI: 0 bar

K = Q: 7.48 = 7.48

System in chemical equilibrium

Ideal mixture of gases Equilibrium constant expression:

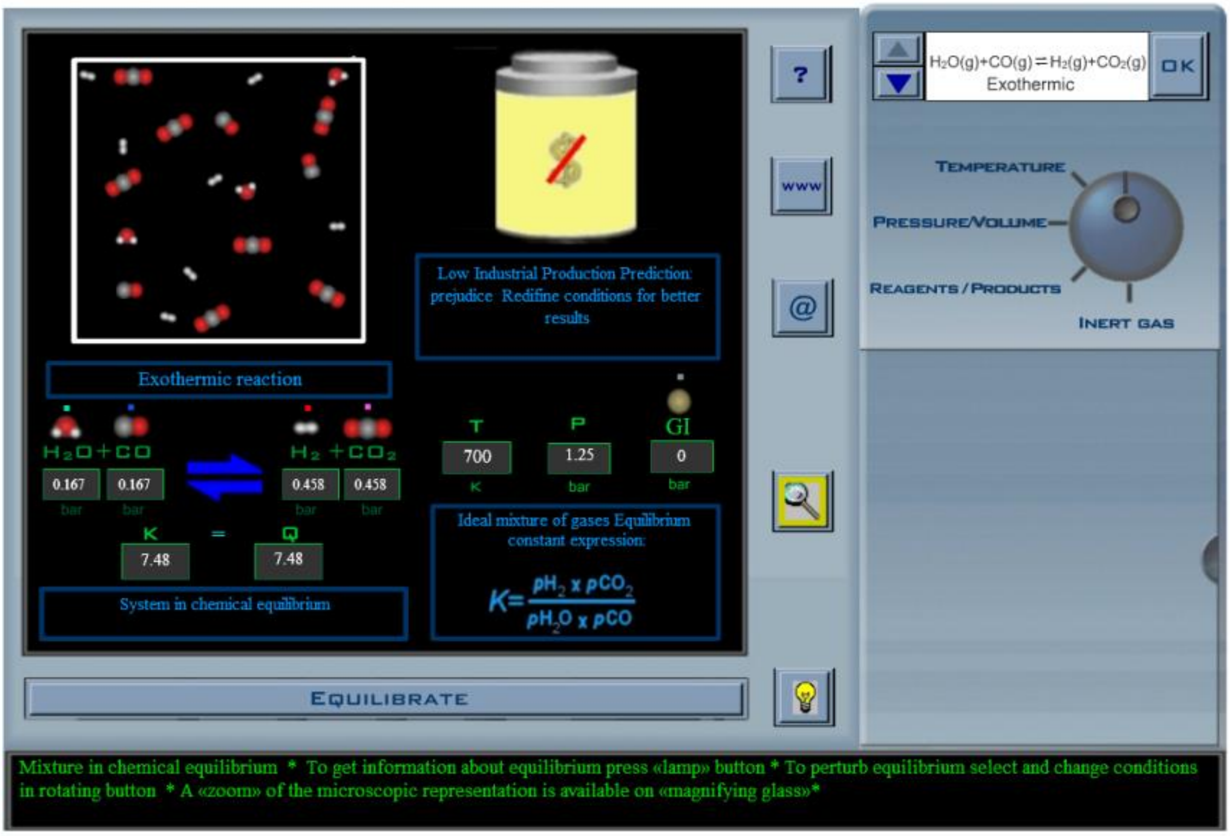
$$K=\frac{pH_2 \times pCO_2}{pH_2O \times pCO}$$

Mixture in chemical equilibrium * To get information about equilibrium press «lamp» button * To perturb equilibrium select and change conditions in rotating button * A «zoom» of the microscopic representation is available on «magnifying glass»*

Figure 5-6 Sequence of images of the simulation, from the moment in which "equilibrate" is pressed until the equilibrium state is established.

In the last image from the previous sequence, the equilibrium state is already established. At this stage, new elements appear on the centre screen. Thus, the symbolic arrow is used to indicate the establishment of an equilibrium state, as well as textual information. The equality between *K* and *Q* is shown by the sign "=" and productivity information is provided in the reactor zone by means of an economic profit metaphor.

By pressing the button identified with a magnifying glass it's possible to switch between the usual microscopic representation, always available, to a closer and more familiar view, using the common molecular models (Figure 5.7).



Low Industrial Production Prediction: prejudice. Redifine conditions for better results

Exothermic reaction

System in chemical equilibrium

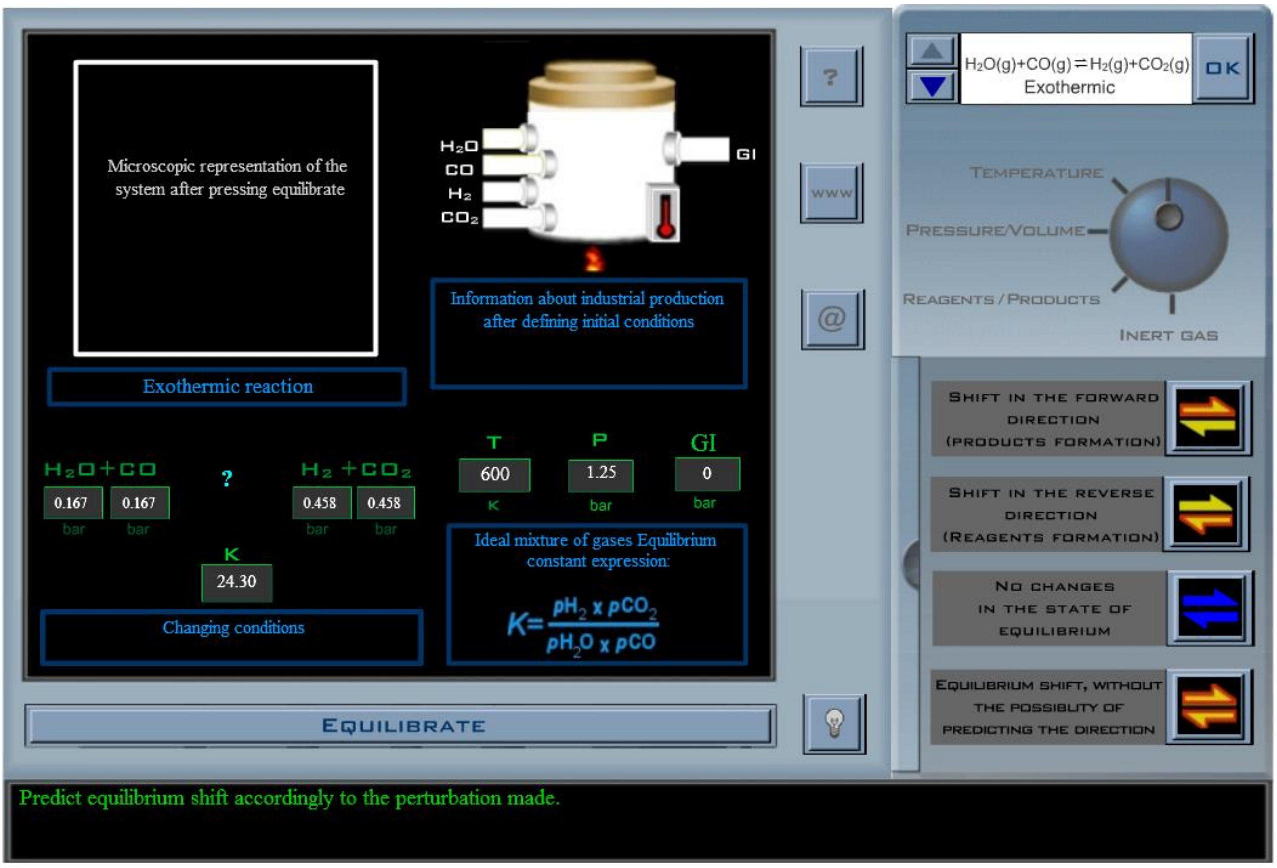
Ideal mixture of gases Equilibrium constant expression:

$$K=\frac{pH_2 \times pCO_2}{pH_2O \times pCO}$$

Mixture in chemical equilibrium * To get information about equilibrium press «lamp» button * To perturb equilibrium select and change conditions in rotating button * A «zoom» of the microscopic representation is available on «magnifying glass»*

Figure 5-7 Zoom element.

Once equilibrium is established, it's possible to introduce disturbances to the reactional system. To do this, simply turn the rotary knob again. An important aspect associated with the disturbance phase is that every time the system is disturbed it's mandatory to predict the effect (Figure 5.8). The information about the correction of the prediction is made available as soon as the new equilibrium state is established. When the prediction is wrong, the user is still informed about the correct prediction.



$H_2O(g)+CO(g) \rightleftharpoons H_2(g)+CO_2(g)$ Exothermic

Microscopic representation of the system after pressing equilibrate

Information about industrial production after defining initial conditions

Exothermic reaction

$H_2O + CO$: 0.167 bar, 0.167 bar ? $H_2 + CO_2$: 0.458 bar, 0.458 bar

K 24.30

T 600 K P 1.25 bar GI 0 bar

Changing conditions

Ideal mixture of gases Equilibrium constant expression:

$$K=\frac{pH_2 \times pCO_2}{pH_2O \times pCO}$$

Predict equilibrium shift accordingly to the perturbation made.

Figure 5-8 Predicting equilibrium shift.

In all simulations there are limitations and certain approximations. Once the programming is done and all the elements present in a simulation are placed, it is time to clearly define the assumptions and simplifications that were the basis of the construction of the same, as well as the differences between real and simulational, in order to avoid the development of misconceptions from lack of information. Basic assumptions and limitations of this resource are listed in Appendix 1.

As seen by the presentation of the prototype, the simulation to be used in this study includes several features suitable for the exploration of chemical equilibrium concepts at all the three levels (submicro, macro and symbolic). The major valences of the simulation are:

1. Demonstrate quantitatively the changes occurring in the system, from the definition of the initial conditions to the establishment of the equilibrium state, as well as variations resulting from disturbances imposed, namely:

    1.1. Allow the comparison between the values of the equilibrium constant and the reaction quotient over time in order to relate to the direction of equilibrium displacement;

    1.2. Monitoring, over time, of the variation of the quantities of the reactive species, in order to understand how this variation progresses until equilibrium is established;

    1.3. Verification of the remaining conditions characterizing the system as: temperature, pressure and quantity of inert gas.

2. Identify the evolution of the system in qualitative terms:

    2.1. Providing information on the direction of displacement of the equilibrium or the establishment of equilibrium state;

    2.2. Informing about the ideality of the system and distinguishing, through the equilibrium constant expression, ideal systems from real systems.

3. Provide a microscopic representation of the system:

    3.1. To give the student a notion of the conditions in which the system is real or ideal and in what way this aspect is notorious in the microscopic representation;

    3.2. Allow concluding whether the system is evolving towards product formation or reagent formation;

    3.3. To be able to illustrate that, regardless of whether quantitative data does not vary in equilibrium, the system does not "stop" at the molecular level.

4. Demonstrate that the influence of an inert gases on Chemical Equilibrium depends on the ideality of the system and that, therefore, there may be an effect on equilibrium under certain conditions.

5. Demonstrate the importance of the theme of Chemical Equilibrium for everyday life and its relationship with technology, namely by referring to industrial production and complementary information about the importance of the systems treated in the simulation.

6. Establish a relationship between microscopic and macroscopic levels by simultaneous representation of features related to both levels.

7. Create a resource with interactivity and student involvement through:

    7.1. The availability of options that determine the results obtained in the simulation, that is, allow the user not only to advance in the simulation, but to define the conditions in which the reaction and the disturbances to be imposed are processed.

    7.2. Developing students' ability to analyze and concentrate, encouraging their engagement with the simulation by predicting the result of their actions.

8. Include the motivational factor:

    8.1. Use of the STS perspective;

    8.2. Placing the student in a challenging role, being able to control industrial productivity.

9. Include complementary information within the simulation, as well as useful links to other resources on Chemical Equilibrium.

10. Explain the limitations and assumptions associated with the construction of the simulation in order to prevent a mismatch between the simulated and the reality.

We have situated the components present in the simulation in the macro, micro and symbolic domains from the triangle of Chemical Equilibrium knowledge space (Figure 5.9). This exercise and the comparison with the triangles from Chapters 2 and 3 facilitates checking the aspects from Chemical Equilibrium teaching covered by the simulation as well as the ones that are left out. A factor worthy of consideration is the adequacy of these resources to the chemistry curriculum and the evaluation of current trends in teaching (Aviram, 2009; Banerjee, 1991b). If we “overlap” the triangles from Figure 5.8 and Figure 3.3 we conclude that there is a resemblance between the aspects covered by the syllabus of Portuguese curriculum and the simulation. The major dissemblance resides in the fact that a gaseous system is selected in the simulation, so partial pressures are preferred instead of concentrations.

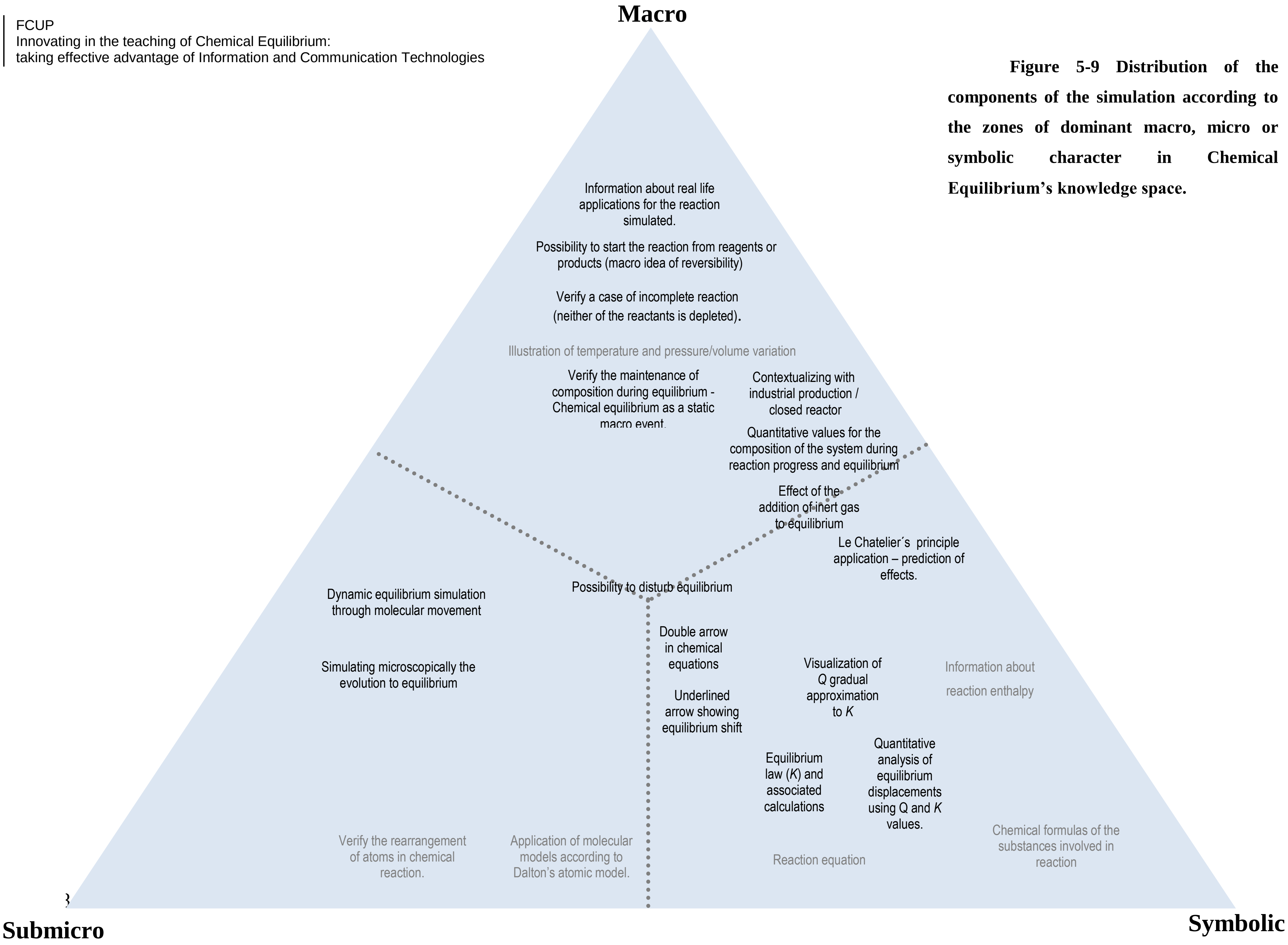


Figure 5-9 Distribution of the components of the simulation according to the zones of dominant macro, micro or symbolic character in Chemical Equilibrium’s knowledge space.

The simulation constitutes only one of the components of the approach that we have designed. The major contribute of the simulation for the process of facilitating abstraction resides in taking advantage from the representative capabilities of computers, as reviewed in Chapter 4, allowing to simulate submicro events and simultaneously provide qualitative and quantitative aspects of equilibrium characteristic of the symbolical level of knowledge, commonly quoted as very abstract. Nevertheless, a point frequently referred in previous chapters is the importance of previous knowledge and the consideration of students' ideas, namely being aware of common misconceptions and conceptual traps. Given the number of studies reporting learning difficulties, it is clear that these should be considered when constructing resources and detected by diagnostic tests (Hackling & Garnett, 1985). Pedrosa and Dias (2000) point out the importance of considering the results of investigations in the design of pedagogical approaches. Literature frequently associates this misconceptions and difficulties with the abstract nature of the concepts in chemistry and specifically in Chemical Equilibrium. So, we consider that in order to facilitate abstraction it is important to guide students in the process of constructing knowledge by planning the approach in order to help minimize the prevalence of these common alternative conceptions.

Exploration guides constitute a mean to support the application of computational simulations. They encompass several tasks, such as answering questions, recording data and reflections. The word "guide" has some behaviorist accent: "although the word "guides" might suggest an overly behaviorist approach to the learning process, we do not intend to deny the importance and the role of constructivism in modern education, especially social constructivism, which is so central in this information society (Paiva & Costa, 2010). Thus, without denying the advantages of constructivism, already mentioned in this dissertation, the scripts may be useful in guiding the student trough the dispersion that might take place during the process of constructing knowledge.

"An effective exploration guide should identify meaningful paths through the resource, show the way (signalling content in addition to navigation) and fix some boundaries, while remaining open and flexible (Paiva & Costa, 2010). Paiva & Costa (2010) presented a set of general characteristics that exploration guides should or may have:

- Manage a balance between constructivist freedom and minimal guidance.
- Offer hints for actions and reflections.
- Include screen-capture images of the program, especially when intended for younger students.
- Incorporate questions to promote discussion.
- Grow increasingly more complex with a guide's questions and tasks.
- Make guides available as printed material or in digital media.
- Make guides customizable and adaptable to various profiles (having several optional questions, for instance).
- Suggest that users keep written records of the exploration, handwritten on paper or in a computer file.

In the case of this simulation, in which the quantity of options and information is high, the existence of guides to support its application becomes an important and perhaps even determining factor of its effectiveness. “A good educational program can be used in either a relevant or an inconsequential way. The human element, the pedagogical experience of a good educator, is always what really matters, even in today's information society. The exploration guides are one possible means of assistance.” (Paiva & Costa, 2010).

The exploration guide was constructed to assist the students through the confrontation of their ideas with the results from the exploration of the simulation, exposing possible misconceptions and favoring their destruction. So, we have constructed an exploration guide based on the review we have made from literature, both considering the usual misconceptions diagnosed in the field of CE and the suggestions made to deal with those resistant ideas, namely the importance of engaging students in conceptual change. The exploration guide used in the study can be consulted in Appendix 2 (original Portuguese version and English version).

The exploration guide initially identifies the purpose of the activity and the location of the application to be exploited. It includes an introduction with the aim of contextualizing the student with the theme and simultaneously increase his curiosity for the exploration of the simulation. Following this information, there are activities to complete with registration spaces and reflection proposals, ending with the incentive to increase knowledge by consulting other sources of information.

The approach also includes a third element, a list of the common difficulties and misconceptions in Chemical Equilibrium based on the compilation made in section 3.3. This auxiliary resource intends to constitute an instrument for the teacher in order for him to be aware of common cognitive traps that the students face when learning this thematic. Instructions about the simulation are also provided to the teacher. The approach is planned to be applied during 90 minutes, in a disposition were each computer is shared by two students.

Figure 5.10 summarizes the main components and the idea on the base of the approach to facilitate abstraction in Chemical Equilibrium learning (FACE) presented in this section. The facilitated abstraction is intended as opposed to "formal abstraction" in which there are no strategies specifically designed for the purpose of facilitating this process of detachment from the concrete. It should be noted that it is not intended to simplify the concept but only to construct a simpler course for its understanding by the student. This strategy may give the student the means to later, in the face of another concept, be able to develop a process of "formal abstraction". Figure 5.9 also points the presence of the teacher along the process, as an essential element to guide the student in the construction of knowledge.

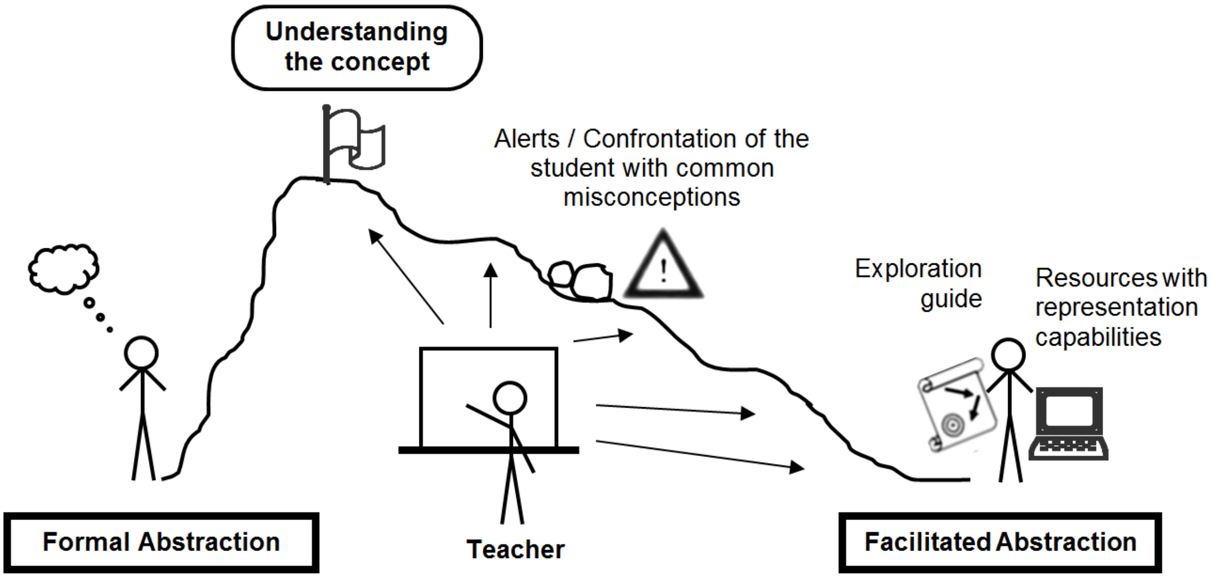


Figure 5-10 Metaphor: formal abstraction / facilitated abstraction

To finish this section we present table 5.3 that recovers the implications for teaching strategies from table 5.2 (reorganized according to their similarity), which we recognize as general "premises for success" in order to facilitate abstraction in the learning process. We analyze how the approach for facilitating abstraction in Chemical Equilibrium learning (FACE) theoretically covers those premises.

Table 5-3 Implications concerning mental process involved in abstraction and FACE approach

Implications for teaching strategies concerning mental process involved in abstraction	*FACE approach*
Clarify simplifications / idealizations associated to a scientific model.	Simulation includes a section were the limitations are exposed, available both to the teacher and the student (Appendix 1).
Expose the failure of common sense ideas in explaining certain events, exposing the need for detachment from sensorial world.	Exploration guide confronts students' ideas with the results from the simulation, guiding them to conceptual change trough questioning, registry and analysis of data.
Expose linguistic and conceptual differences from everyday language.	Face strategy uses the terms common in Chemical Equilibrium, the teacher play an essential role in the confrontation with different meanings in everyday language.
Encourage students to reflect on events and predict responses in order to expose relationships. Promote student's **active learning**.	Exploration guide proposes a written reflection after each activity and the fact that two students share the same computer also encourages the exchange of opinions and ideas. The manipulation of conditions and the need to predict events (in the simulation) as well as the concretization of the activities proposed in the exploration guide contribute to the active involvement of the student in the learning process.
Minimize the absence of concrete experiences **using representations that support the ideas**. **Appeal to analogies** in order to establish metaphors with more concrete concepts. **Use simulations to represent/interact with models**, assisting mental abstraction and analogical inferences.	The simulation includes several analogies with concrete objects and intuitive representations: analogy between the reactional system and an industrial reactor, temperature changes manipulated in a thermometer, global appearance of the simulation as a control panel, colored dots in movement to represent different species and events at the submicro level…
Teacher must guide the student in the process from concrete to abstraction.	FACE approach predicts an active role of the teacher in guiding the student trough the construction of knowledge.
Should be given numerous opportunities to **relate the three representations** so that multiple linkages are formed in long-term memory. **Provide different explanations** for the same concept. Follow the **multiple representation** principle**.** **Relate different levels of description of a concept (macro, micro, symbolical).** **Expose relations between different levels of description** like macro and micro scale, so that students can construct unified explanation of phenomenon.	The simulation reunites concepts predominantly belonging to any one of the levels in a single resource, allowing simultaneous illustrations of the macro, submicro and symbolic evolution of the system. Questions in the exploration guide relate knowledge from the three levels represented in the simulation. The simulation presents representations of the events that lead to equilibrium (at macro, submicro and symbolic levels) supporting the ideas of the scientific model.

Implications for teaching strategies concerning mental process involved in abstraction	***FACE approach***
Establish a sequence to approach the different levels of chemical knowledge. **Present the convenience/evidence for extending a concept to new domains.** Study the familiar macroscopic world first, and then explain that world using the particulate nature of matter. In this way **new concepts are anchored on the concepts of a pre-existing network** in long term memory.	FACE approach predicts that the concepts have been previously introduced to the student in a sequence established by the teacher and the syllabus of the discipline.
Help to mobilize previous abstractions and consider them as the basis for new abstractions during the design of teaching strategies. **New concepts need to be anchored on the concepts of a pre-existing network in long term memory.**	A list of difficulties and misconceptions, in which several are related to prerequisite concepts, as well as the consideration of these difficulties in the design of the exploration guide constitute a concern with the need to anchor the concepts in previous knowledge.
Importance of **applying concepts in context,** so that knowledge acquires real meaning. Complete a cycle beginning with detachment from events to deal with ideas, which are later used to explain those events.	Information about the reaction and the context of industrial production is used in the simulation.

Chapter 6 - Using FACE in the Classroom

6.1. Problematic, goals and investigation hypotheses

The central problematic of this dissertation is to understand how to make an effective use of the potential of ICT for the teaching of Chemical Equilibrium. In this way, this project involves the development of actions and studies in order to contribute to a better use of ICT in the teaching of Chemical Equilibrium. The expression "a contribution" appears here to emphasize that it is not a matter of discovering the only way, but rather of obtaining guidance on a possible course. Also, there is no pretention to arrive at miraculous solutions, which will solve all the problems in the teaching of this subject, but only to minimize some of the difficulties. Based on what has been mentioned in previous chapters, as a result of a bibliographical review and previous experience of this work group on the theme, the arrival to this problematic comes from the following findings:

- Thematic composed of abstract concepts predisposing to the application of ICT based approaches, which have recognized potential in the ability to make visible representations of what is not directly observable;

- Availability of resources contrasts with learning difficulties in Chemical Equilibrium, demonstrating the importance of continuing to develop actions in this area;

- References warn about the importance of the strategies used in the construction of ICT and the pedagogical approach followed in its application;

- Development of new technologies of representation / interaction, dissemination of Web 2.0 and better technological equipping of the schools in the last years;

- Increase in the time spent by young people on the computer and online, imposing the Internet as a means of informal education of science.

The main purpose of this project is to innovate in the teaching of Chemical Equilibrium, by taking effective advantage of the potential of ICT. Underlying this central purpose, the following objectives were defined:

- Collect information about "good practices" involving the use of ICT in the teaching of Chemical Equilibrium, in order to gather a theoretical framework of action in this area;

- Through previous literature review, build an ICT based approach aimed at implementing the process of facilitated abstraction in the learning of Chemical Equilibrium;

- Obtain guidelines for the use of computational resources in the teaching of Chemical Equilibrium, by studying the materials produced in a classroom context, describing advantages and difficulties throughout the process;

- Reformulation of the FACE approach and the resources that constitute it through implications taken from the study results;

- Make FACE approach available online (in Portuguese and English versions) and disseminate the approach built – trough Web 2.0 platforms and publications in international journals;

- Promote the development of teachers' capacities for the use of ICT.

According to these objectives, with the innovation to be introduced in the teaching of Chemical Equilibrium we aim to implement the process of facilitated abstraction by the use of an ICT based approach, the diversification of pedagogical resources and the involvement of teachers in the use of ICT approaches for the teaching of Chemical Equilibrium.

The FACE approach built within this project was developed in the framework of the chemistry curriculum for high school chemistry and supported by findings and indications from previous studies. We have considered the specific nature of chemistry, namely the abstract nature of many concepts (Barke & Wirbs, 2002; Gabel, 1993, 1999; Jensen, 1998; Johnstone, 1982, 1991, 2000; Potgieter et al., 2008; Sirhan, 2007; Sjöström, 2007; Taber, 2001; Tsaparlis, 2001), difficulties found in the teaching of CE (Azizoğlu et al., 2006; Banerjee, 1995; Bergquist & Heikkinen, 1990; Cheung, 2009; Erdemir et al., 2000; Hackling & Garnett, 1985; Huddle et al., 2000; Maskill & Cachapuz, 1989; Özmen, 2008; Solaz and Quílez, 2001; Tyson et al., 1999; Van Driel et al., 1999; Van Driel & Gräber, 2002; Wilson, 1998) and research on the use of ICT in science education and particularly CE (Hameed et al., 1993; Huddle et al., 2000; Karpudewan et al., 2015; Mintzes et al., 1998; Paiva et al., 2002; Russell et al., 1997; Sandberg & Belamy, 2003; Sarıçayır et al., 2006; Sprague et al., 2005). Thus, it is expected that the application of the approach in context, the classroom, reveals itself as the right choice for a facilitated abstraction. Thus, a hypothesis is placed *a priori* in the realization of this investigation:

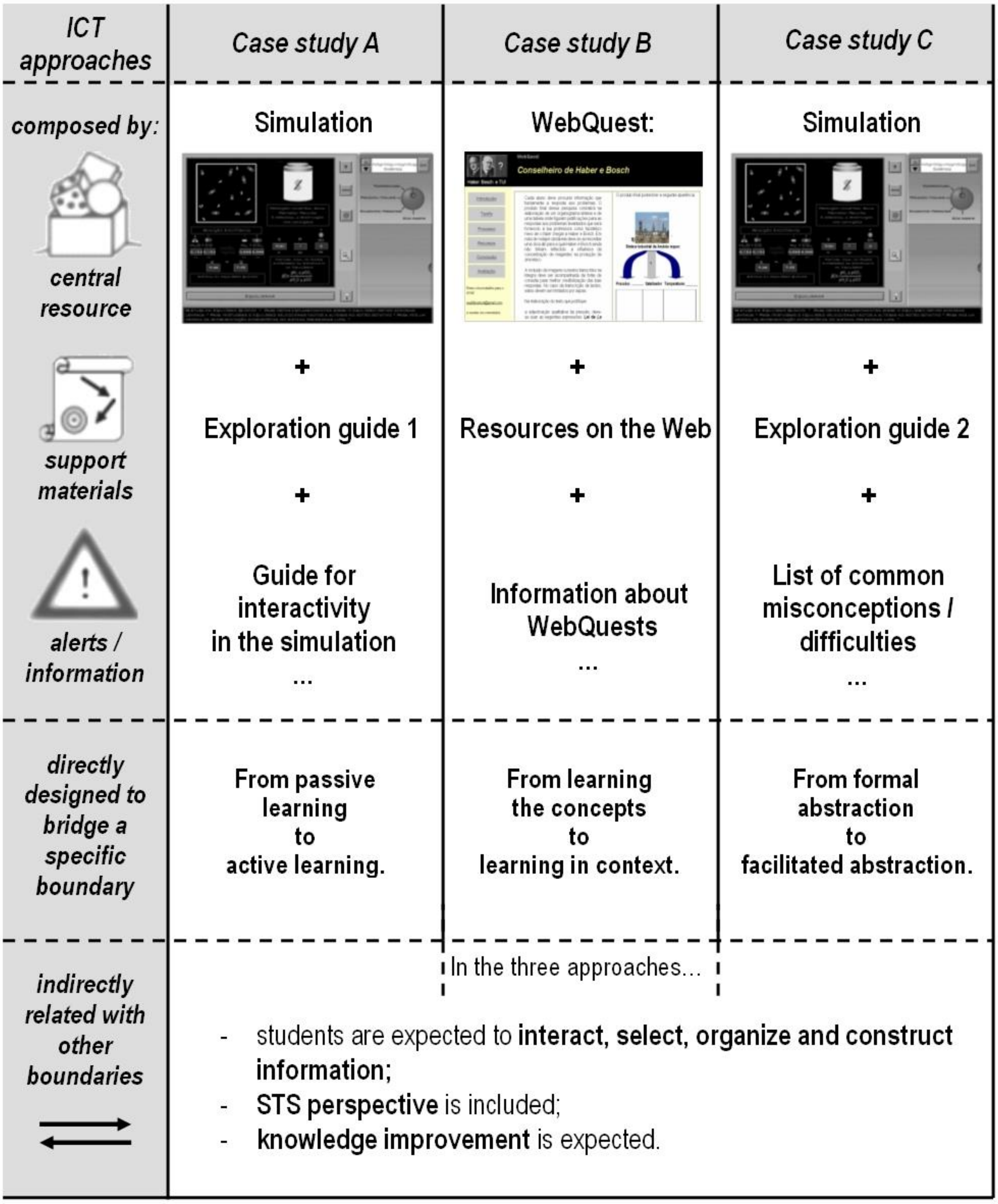
**"FACE promotes facilitated abstraction in a classroom context,
and there is a practical relevance of the theoretical assumptions
that served as a basis for the construction of the same."**

However, as can be seen from the method used in this research - the case study (presented in the next section), there is openness to new hypotheses throughout the process.

6.2. Methodology

Carmo and Ferreira (1998) point out that before starting any research in education there are two issues that need to be addressed: the question of available information and the question of time management. In this case, the working group was concerned with a temporal management that would allow synergies with the European CROSSNET project, thus benefiting from the exchange of knowledge with an experienced group and opportunities for the dissemination of the work (Fonseca & Paiva, 2007; Fonseca et al., 2008; Paiva and Fonseca, 2009; Paiva & Fonseca, 2012). The general theme of the CROSSNET was "crossing boundaries in the teaching of science", which is compatible with the work area of the Portuguese group (the Teaching of Chemical Equilibrium) and specifically with the importance of transposing the formal abstraction barrier associated with this PhD project. This scenario has made it evident that it was important to define a common line of research with this European project.

As already mentioned, the CROSSNET project has passed through the development of innovative projects and later applications of case studies in order to better understand the events or phenomena involved. The Portuguese proposal focused on the construction and study of the application of ICT based approaches, which were developed with the purpose of transposing barriers in the teaching of Chemical Equilibrium. Thus, three case studies were included in the national study, associated with the use of specific pedagogical approaches: facilitated abstraction, in-context learning and active learning. These cases focused on the different components of the global phenomenon (transposing barriers in the teaching of Chemical Equilibrium), constituting units that can be designated as embedded cases (Yin, 1994). In this doctoral project, one of the cases included of the Portuguese participation in the CROSSNET was given additional in-depth and continuity.



ICT approaches	*Case study A*	*Case study B*	*Case study C*
composed by: *central resource*	**Simulation**	**WebQuest:**	**Simulation**
support materials	+ **Exploration guide 1**	+ **Resources on the Web**	+ **Exploration guide 2**
alerts / information	+ **Guide for interactivity in the simulation** ...	+ **Information about WebQuests** ...	+ **List of common misconceptions / difficulties** ...
directly designed to bridge a specific boundary	**From passive learning to active learning.**	**From learning the concepts to learning in context.**	**From formal abstraction to facilitated abstraction.**
indirectly related with other boundaries ⇄	In the three approaches… - students are expected to **interact, select, organize and construct information;** - **STS perspective** is included; - **knowledge improvement** is expected.		

Figure 6-1 – Embedded cases in the Portuguese contribution to CROSSNET project (Paiva & Fonseca, 2012).

The case study methodology is particularly appropriate when the researcher seeks answers to questions such as "how?" and "why?", when aiming to find interactions between relevant factors, when the purpose is to describe or analyze the dynamics of a contemporary phenomenon, program or process in its context (Yin, 1994). We can summarize the main ideas of Yin about case study methodology (Kohlbacher, 2006):

- investigates a contemporary phenomenon within its real-life context, especially when the boundaries between phenomenon and context are not clearly evident;

- copes with the technically distinctive situation in which there will be many more variables of interest than data points, and as one result relies on multiple sources of evidence, with data needing to converge in a triangulating fashion, and as another result benefits from the prior development of theoretical propositions to guide data collection and analysis.

In this work, an innovative approach was developed, which had not yet been tested in its context. In this way, it is relevant to investigate "how it works", to know its advantages and weaknesses, as well as the factors that influence it. Positive feedback is expected from the application of this approach, given that it was constructed on the basis of a theoretical frame of reference. However, the central aim of this case study is not to conclude whether there is a positive or negative impact, but above all to understand "how" and "why" such impact happens. “To gain a sense of science teacher pedagogy with computer simulations, the researcher requires detailed accounts of how teachers accomplish this and the relationships among pedagogy, technology, content, and learners. Such research is better captured with case studies involving careful teacher observation and interview rather than larger survey research alone.” (Khan, 2011).

Yin (1994) states that case studies can be essentially exploratory (preliminary information), descriptive (explaining) and analytical (confronting their subject with existing theory and / or developing new theory). These purposes fit this case, since it is intended to explore the interaction between the various elements that make up FACE approach (resources, support materials, teacher alerts ...), describing how they work with regard to the promotion of facilitated abstraction, explaining what conditions confer it usefulness and confirm the theoretical premises that served as its basis.

At the end of this study, it is expected to obtain guidelines / recommendations for the implementation of ICT in the teaching of Chemical Equilibrium and data for the reformulation of the specific approach developed. More than conclusions, these guidelines and recommendations are hypotheses to be tested in possible later investigations, a characteristic point of the case study methodology (Yin, 1994). This aspect is in agreement with the objective of understanding the event under study and at the same time developing more generic theories about the phenomenon observed (Fidel, 1992 cited by Araújo et al., 2006).

There is some suggestion that the case study method is increasingly being used and with a growing confidence in the case study as a rigorous research strategy in its own right (Kohlbacher, 2006). The case studies can have a well-established theoretical orientation that supports the formulation of the respective questions (Ponte, 2006). It was on the basis of the aforementioned theoretical framework that the guidelines for this study were established, with emphasis on the "facilitating abstraction". We formulated the following research questions:

- **How does FACE approach work in promoting facilitated abstraction in the classroom context?**

- **Is the practical relevance of the theoretical assumptions underlying the construction of FACE approach confirmed?**

- **What are the conditions, in the case under study, that promote facilitated abstraction by the use of computational resources?**

6.3. Data collection

Although the selection of the sample is extremely important, Stake (1995) quoted by Araújo et. al. (2006) alerts that research in a case study is not based on sampling. By choosing the "case" the researcher establishes a logical and rational guiding line that will guide the whole process of data collection (Creswell, 1994 cited by Araújo et al., 2006). According to Bravo (1998) cited by Araújo et. al. (2006), the constitution of the sample is always intentional, based on pragmatic and theoretical criteria, to the detriment of probabilistic criteria. The same author identifies six types of samples that can be used in a case study, the convenience sample being among the possible ones. Benbasat et al (1987) cited by Araújo et al (2006) also refers that experimental methods of control or manipulation are not used in case studies and that the investigator doesn’t need to specify the set of dependent and independent variables in advance.

The participants of our study were chosen by convenience. In this type of sample a group of volunteers is used (Carmo & Ferreira, 1998). The results cannot be generalized to the population to which the convenience group belongs, but valuable information can be obtained if used with due caution and reservations (Carmo & Ferreira, 1998). The sample was a group of secondary school students (25 students), from the Science and Technology grouping, at the Secondary School of Santa Maria Maior in Viana do Castelo.

The researcher simultaneously assumed the role of teacher of the class participating in the study, taking advantage from the attribution of a class from the 11th grade to her: the curricular period in which the theme of Chemical Equilibrium is taught. This overlap of functions has strengths such as the particular sensitivity to details and the ability to reorient research. However, it also presents weaknesses such as the possible interference of ideas and the contagion of enthusiasm. In an attempt to minimize the influence of the latter in the interpretation of data, multiple data collection instruments were used. Table 6.1 presents a brief characterization of the sample.

Table 6-1 - Characterization of the sample.

School	Secondary School of Santa Maria Maior
Location	Viana do Castelo, Portugal.
Study year	2008
School year	11th grade
Number of students	25
Distribution by gender	9 girls 16 boys
Average Age	16 years
Results	Number of students: A) retained in the previous school year: 0 B) with retentions along their school path: 1 The class is globally composed by interested students with a medium to good performance.
Performance in the discipline of Physics and Chemistry	A) negative result in the previous year: 1 B) negative result at the end of this academic year: 1 C) repeating the discipline: 2 (1 of them by option for classification improvement).
Other information	The generality of the students shows a good attendance. The behaviour of the students was reasonable to good, with some tendency of the group for losing focus and dispersing.

Case study's unique strength is "its ability to deal with a full variety of evidence - documents, artifacts, interviews, and observations" (Yin, 1994). This ideas is reinforced by other authors (Araújo et al., 2006). In this doctoral project multiple data sources were used. Thus, several "measures" of the same phenomenon are obtained, creating conditions for triangulation of the data, during the analysis phase (Araújo et al., 2006; Yin, 1994). The use of various sources of data collection contributes to the internal validity of a study (Descombe, 1998, Yin, 1994), not being only a construction of the more or less fertile imagination of the researcher (Araújo et al., 2006). Araújo et. al. (2006) report that although the most common data collection methods in a case study are observation and interviews, no method can be discarded. The methods of collecting information should be chosen according to the task to be accomplished (Bell, 1989 cited by Araújo et al., 2006).

In order to understand the operation of our ICT approach with regard to the promotion of facilitated abstraction, data collection instruments passed through observation, documentation and questionnaires, respectively:

- Observation; interventions and opinions of students;
- Answers to the Exploration Guide;
- Pre-test and post-test.

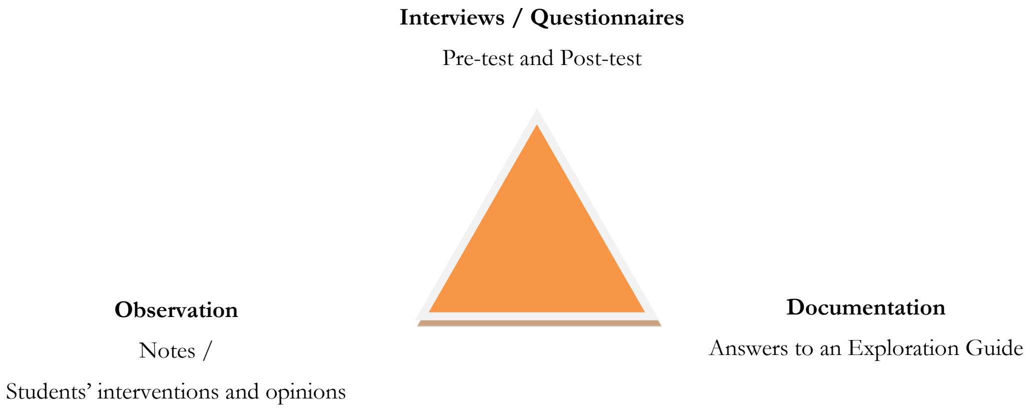


Figure 6-2 Instruments for data acquirement

The use of FACE approach in the classroom assumes that CE is previously introduced by what we call "regular" teaching methods. The classroom for the application of FACE approach was not the usual classroom for the lesson. An exchange was made in order to benefit from a classroom with 11 computers arranged in a U shape, allowing the possibility of each two students sharing a computer (in a few cases three students had to share the same computer). The computers were somewhat “old” and of limited capacity, but allowed to use the simulation without major technical problems except for some delay in beginning the activity due to the time needed to load windows, connect to the internet…

Next we present the time sequence of the procedures performed in the classroom context (Figure 6.3) and some photographs of the application of FACE in the classroom (Figure 6.4).

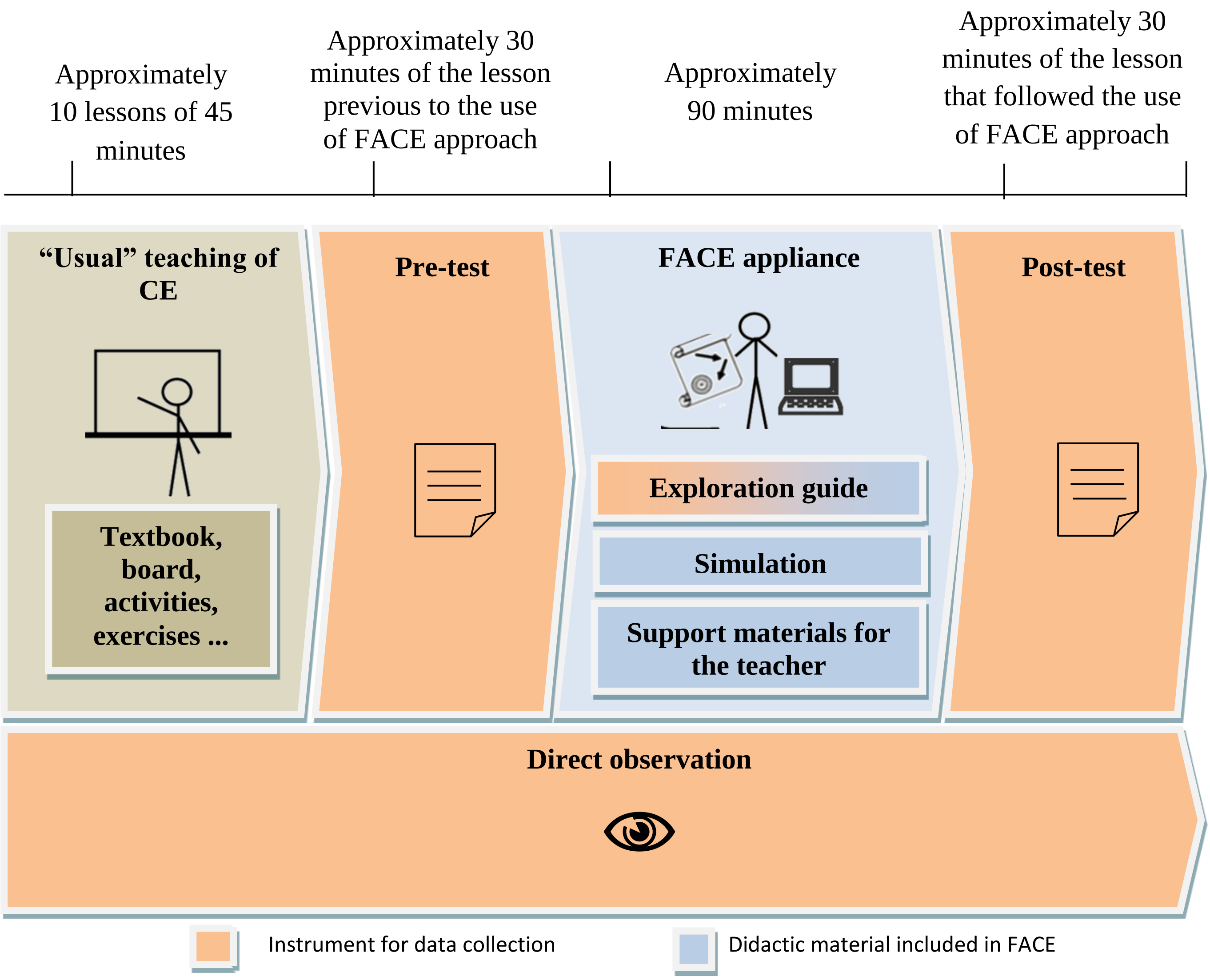


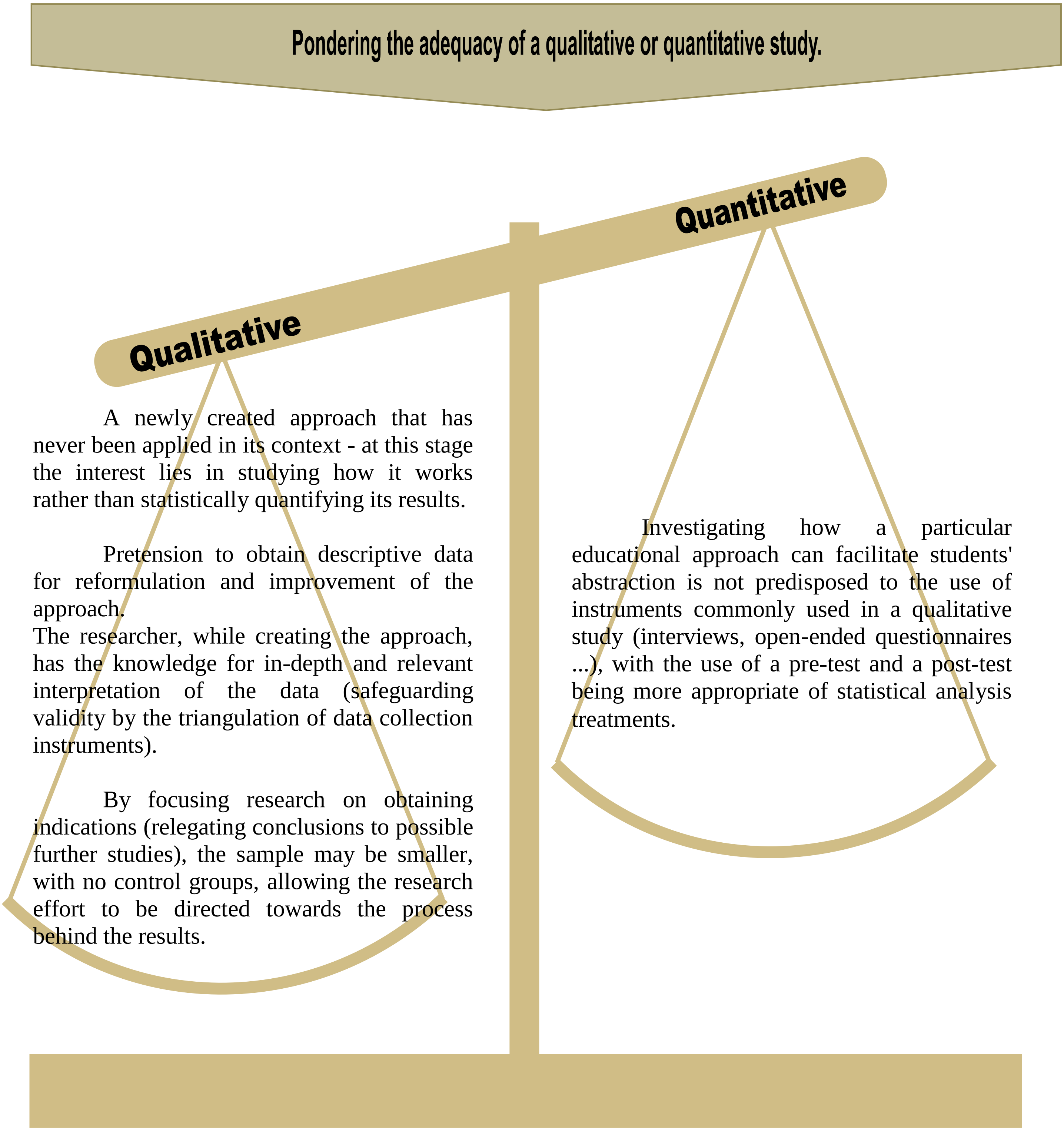
Figure 6-3 – Time sequence of the procedures performed in the classroom context

Figure 6-4 - Applying FACE approach in classroom context

6.4. Data treatment

The case study is commonly considered a possible methodological design within qualitative methods. However, there are authors who argue that the case study can be included in the mixed-type research plans (Araújo et al., 2006; Ponte, 2006). In our investigation, since the general objective is to understand what factors influence and contribute to the process of facilitated abstraction by the use of ICT, this study has a fundamentally qualitative framework. The central purpose is not only to know if there were modifications in the students' ability to deal with CE concepts, but rather to understand where and why these changes occur. In order to establish relationships that allow an understanding about how the FACE approach affects the abstraction process (what difficulties arise, where they are revealed, strengths and weaknesses ...) the various sources of data collection are considered.

The fact that we intend to explore the behaviour of the approach in a classroom context is in agreement with the use of a qualitative study that tries to perceive and describe more than to count or just verify. However, to understand how FACE approach affects abstraction abilities we will analyse the presence of common misconceptions, since, as we have seen in chapter 5, references point a relation between learning difficulties and the abstraction abilities necessary to understand formal concepts. Diagnose of alternative conceptions appeals for the use of specific questions. Interviews or free questionnaires could leave unexposed the aspects and relations that we intend to investigate. So, we have used a pre-test and a post-test, instruments that are usually more associated to quantitative studies. They are imposed by the specificity of the knowledge that is sought: to identify the presence or absence of learning difficulties inherent to the process of abstraction. Nevertheless, the analysis of the tests will be centred in describing the relation between the results and the content of FACE approach more than in just quantifying the improvements, thus justifying the use of this instruments in a study with qualitative character. In figure 6.5 we ponder the adequacy of qualitative / quantitative methods of analysis, with the balance swinging clearly in favour of a qualitative study.



Pondering the adequacy of a qualitative or quantitative study.

A newly created approach that has never been applied in its context - at this stage the interest lies in studying how it works rather than statistically quantifying its results.

Pretension to obtain descriptive data for reformulation and improvement of the approach.
The researcher, while creating the approach, has the knowledge for in-depth and relevant interpretation of the data (safeguarding validity by the triangulation of data collection instruments).

By focusing research on obtaining indications (relegating conclusions to possible further studies), the sample may be smaller, with no control groups, allowing the research effort to be directed towards the process behind the results.

Investigating how a particular educational approach can facilitate students' abstraction is not predisposed to the use of instruments commonly used in a qualitative study (interviews, open-ended questionnaires ...), with the use of a pre-test and a post-test being more appropriate of statistical analysis treatments.

Figure 6-5 Pondering the adequacy of a qualitative and quantitative study.

Cassel and Symon (2004) highlight the characteristics of a qualitative research:

"a focus on interpretation rather than quantification; an emphasis on subjectivity rather than objectivity; flexibility in the process of conducting research; an orientation towards process rather than outcome; a concern with context—regarding behaviour and situation as inextricably linked in forming experience".

In the course of the last century (especially the second half of it), the development of qualitative methods showed impressive advances and results, thus helping to gain more acceptance not only in the field of social research (Kohlbacher, 2006). A careful description of the data and the development of categories in which to place behaviors have proven to be important steps in the process of analyzing the data.

The process of data analysis to be carried out in this study includes the technique of content analysis. The simplest type of analysis consists of counting the numbers of occurrences per category (assuming there is a relationship between frequency of content and meaning) (Kohlbacher, 2006). Qualitative content analysis, as developed by Philipp Mayring, tries to overcome these shortcomings of classical quantitative content analysis by applying a systematic, theory-guided, approach to text analysis using a category system (Kohlbacher, 2006). Berelson (1952, 1968), quoted by Carmo and Ferreira (1998), defines content analysis as a research technique that allows an objective and systematic description of the manifest content of communications for the purpose of interpretation.

Mayring (2000) refers that one of the possibilities to define the categories of analysis is prior formulated, theoretical derived aspects of analysis, bringing them in connection with the text. If the research question suggests quantitative aspects (e.g. frequencies of coded categories) can be analyzed. Categories and a coding scheme can be derived from three sources: the data, previous related studies, and theories (Zhang & Wildemuth, 2005).

From a qualitative analysis perspective, balancing the pre-test and the post-test results constitutes a mean to gather data for the next stages of analysis and not an end itself. The results from this stage of analysis are then triangulated with the answers to the exploration guide and the direct observation of the students. This procedure, in turn, provide good indicators about the reasons why changes occur, revealing that our focus resides in interpretation rather than quantification.

The pre-test and post-test were elaborated based on a bibliographical review, including typical diagnostic questions of alternative conceptions (Appendix 3). In favor of diminishing null responses, there is the fact that this evaluation is important for the respondents (Carmo & Ferreira, 1998) because it is one of the subject matters of their evaluation in the discipline of Physics and Chemistry.

In our case we have defined three dimensions of analysis:

1. **Difficulties in the learning of CE;**

2. **Familiarization with CE language;**

3. **Participation/ Interest revealed by the students.**

The dimensions were selected considering the questions and hypothesis we have posed in the beginning of the study. Thus, in order to acquire information about FACE approach, namely the conditions that facilitate abstraction and the practical relevance of the theoretical assumptions on the base of its construction, we analyze learning difficulties, the familiarization with CE language and the interest students reveal in the activities.

As already referred, in this investigation it was previously considered a set of theoretical assumptions which included the common misconceptions in CE and their relation to the process of abstraction. So, the categories of the first dimension of analysis are a set of difficulties/misconceptions in Chemical Equilibrium which are possible to detect with the appliance of the pre-test / post-test we have designed. In this type of analysis categories are defined at *priori* and so are the criteria (indicators of correspondence to a given category). The indicators are defined as the combination of answers to the pre-test and post-test that reveal the presence or absence of the difficulty/misconception.

For the second dimension of analysis we search in the open answers to the pre-test, post-test and exploration guide indicators of the presence of language characteristic connected to the CE model, in order to understand if and how the approach is able to develop this type of knowledge in the students.

The final dimension of analysis consists in searching for indicators of interest and motivation in the various elements for data collection, including the notes from the observation made throughout the study.

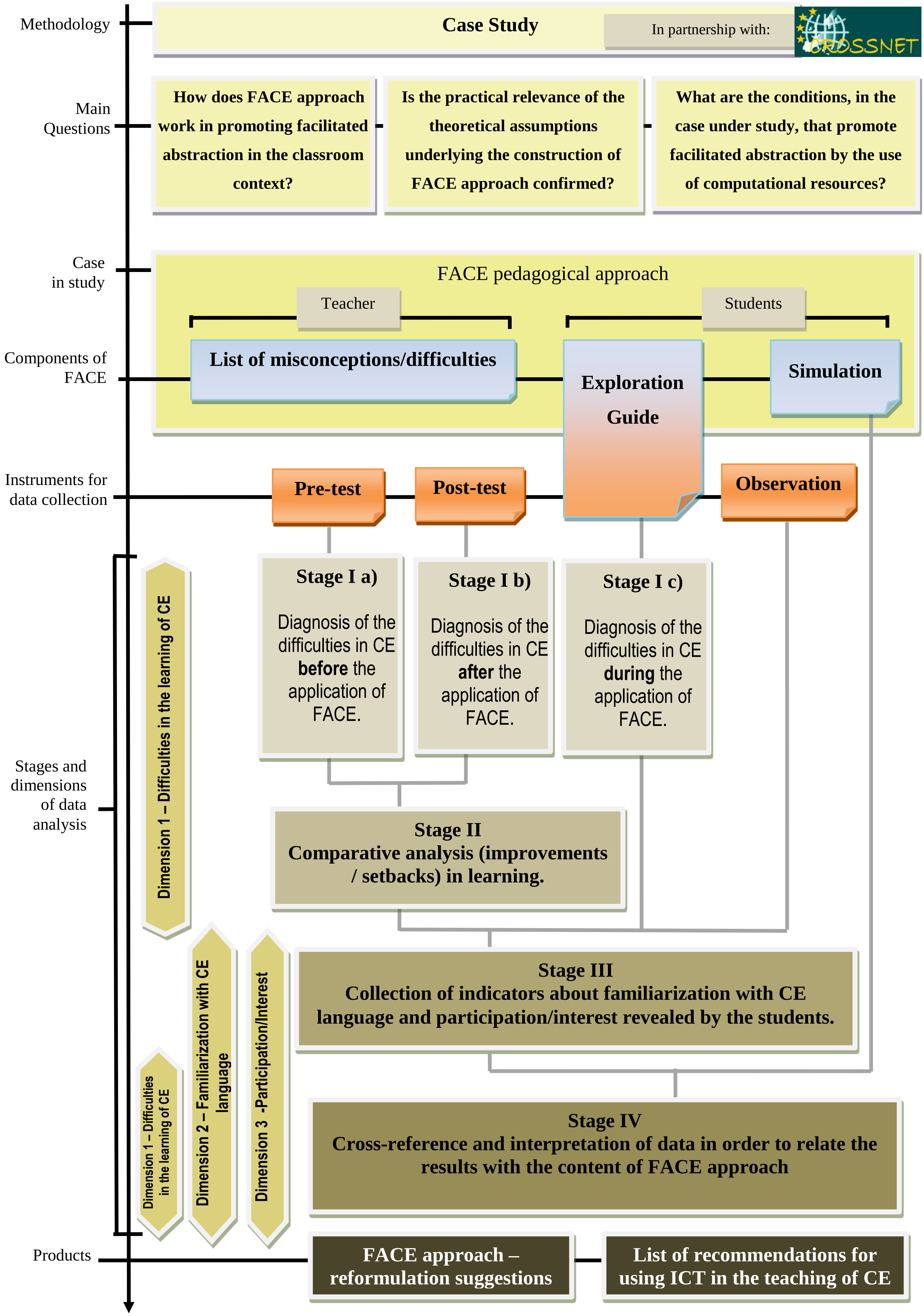
In order to cover the 3 dimensions, the process of analysis also involves 4 stages:

- **Stage I - Diagnosis of the difficulties in CE throughout the study;**
- **Stage II –Comparative analysis (improvements / setbacks) in learning;**
- **Stage III - Collection of indicators about familiarization with CE language and participation/interest revealed by the students.**
- **Stage IV- Cross-reference and interpretation of data in order to relate the results with the content of FACE approach.**

It is important to remark that the conclusions appear as merely indicative, without the intention of establishing direct cause and effect relationships or generalizations. However, it is hoped that the information resulting from this study will be a guideline for action in this area of research in education. Table 6.2 presents a summary of the methodology followed in this PhD project. Figure 6.6 schematizes the case study conducted including the stages of analysis and the instruments used at each step.

Table 6-1 - Methodology followed in the case study

Qualitative Methodology	Case Study	• Is it intended to answer a question like "how?" - "How does FACE approach work with regard to promoting facilitated abstraction in CE learning?" • It aims to increase knowledge about an innovative approach in its context. • Partnership with the CROSSNET project.
Instruments for data collection	Pre-test and post-test	• They are imposed by the specificity of the knowledge that is sought: to identify the presence or absence of learning difficulties inherent to the process of abstraction. • Advantage of not being easily controllable by the researcher.
	Exploration guide	• Simultaneously an instrument and a pedagogical element of the approach, favouring the inference of relations between the results and the process.
	Observation	• For triangulation of data sources and collection of additional information.
Data analysis	Content Analysis	• Pre-test / post-test comparative analysis (categorized according to theoretical assumptions) as a means to achieve the purpose of understanding the operation of the approach and not as the end itself. The learning improvements / setbacks are triangulated with the other elements in a qualitative perspective to obtain information about the performance of the approach regarding the facilitated abstraction in CE learning.



How does FACE approach work in promoting facilitated abstraction in the classroom context?

Is the practical relevance of the theoretical assumptions underlying the construction of FACE approach confirmed?

What are the conditions, in the case under study, that promote facilitated abstraction by the use of computational resources?

Stage I a)

Diagnosis of the difficulties in CE **before** the application of FACE.

Stage I b)

Diagnosis of the difficulties in CE **after** the application of FACE.

Stage I c)

Diagnosis of the difficulties in CE **during** the application of FACE.

Stage II
Comparative analysis (improvements / setbacks) in learning.

Stage III
Collection of indicators about familiarization with CE language and participation/interest revealed by the students.

Stage IV
Cross-reference and interpretation of data in order to relate the results with the content of FACE approach

FACE approach – reformulation suggestions

List of recommendations for using ICT in the teaching of CE

6.5. Presenting the results

6.5.1. Stage I - Diagnosis of the difficulties in CE throughout the study

As exposed in previous section, the categories and indicators for the first dimension of analysis (difficulties in the learning of CE) were previously defined according to the learning difficulties and misconceptions covered in the pre-test and post-test. These difficulties and the questions from the tests were, in turn, selected based on references about common difficulties in CE, the knowledge intended to be constructed in the regular courses of chemistry (at a secondary school level) as well as considering the content of the simulation and the exploration guide. English version of the tests are available in Appendix 3 and the original tests filled by the students follow in attachment in digital version.

In the first stage of analysis each instrument of data collection is treated individually:

- **Stage I a) - Diagnosis of the difficulties in CE before the application of FACE approach (pre-test).**

- **Stage I b) - Diagnosis of the difficulties in CE after the application of FACE approach (post-test).**

- **Stage I c)- Diagnosis of the difficulties in CE during the application of FACE approach (exploration guide).**

For each sub stage, we present the categories and the indicators. The pre-test and the post-test are similar in content, nevertheless they constitute two different versions (indicators diverge) in order to minimize the effects of students answering in function of memorizing the previous pattern.

In order to analyze students' answers to the pre-test and post-test we inscribed data in an excel file, which also follows in attachment to this dissertation. We present the results obtained for the pre-test and the post-test in the form of two separated tables. We have chosen a colorimetric presentation of the results, where red indicates the presence of the indicator for the category (student reveals the difficulty), green means the absence of the difficulty (student reveals the absence of difficulty) and yellow is for inconclusive results.

For the exploration guide, indicators are related to the registries, answers and reflections/conclusions that students are asked to complete during the activity. For some categories, it is only predicted that students perform the actions proposed in the exploration guide which depend on specific components of the simulation, so no registries or answers are expected. In these cases no indicators for that category are collected from the exploration guide, being the results dependent on further analysis and triangulation of data performed in posterior stages, which we will present later. English version of the exploration guide is available in Appendix 2 and, as with the pre/post-test, the original exploration guides filled by the students are available in attachment in digital version.

The results from the exploration guide are also presented in the format of a table that summarizes the frequency of the indicators for each category. Again we present a colorimetric scale for the results. In this case the colors are defined according to the percentage of correct answers to the exploration guide: red means that 50% or less of the students answered correctly, yellow means that 50% to 75% of the students answered correctly and green means that more than 75% of the students answered in correct fashion. An excel file was also previously used to insert the data from each student concerning the exploration guide.

Table 6-2 Pre-test pre-analysis: definition of categories and identification of indicators for the dimension of analysis 1.

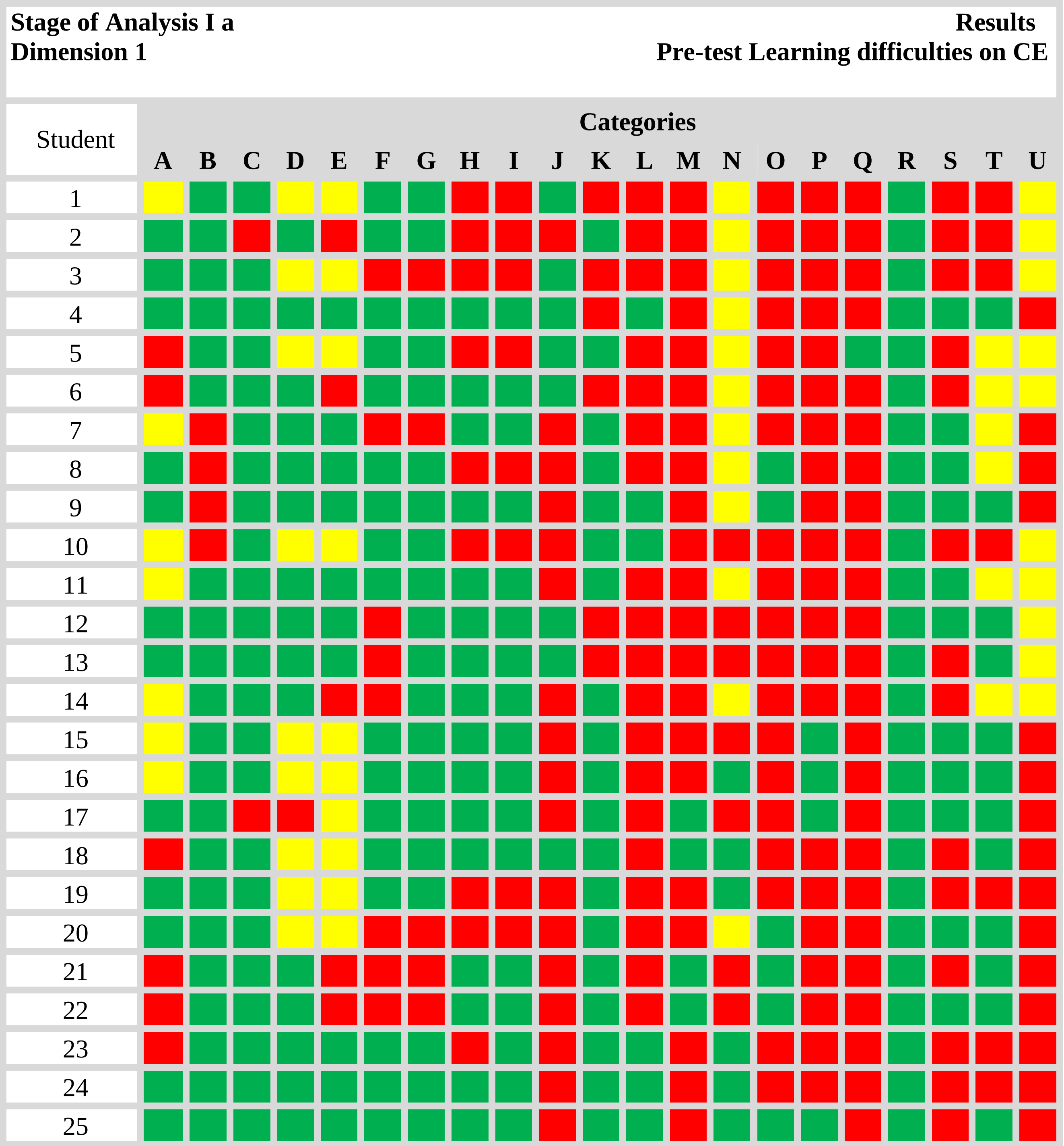
Question	**Unity** (Topic under study)	**Category** (Difficulty / misconception to be detected)		Indicator of the presence of the category (the student manifests the difficulty)	Indicator of the absence of the category (student reveals the absence of difficulty)	Inconclusive answer
1. Set of options I	Chemical Equilibrium state	**A**	**The concentration of reagents and / or products changes during equilibrium state.**	Check option 5 and do not check option 2	Check option 2 and do not check option 5	Check options 2 and 5 or do not check any of these options.
		B	**The reaction rate decreases in equilibrium state**	Check option 3	Do not check option 3	________
		C	**Starting from the reactants a different equilibrium state is obtained, than starting from the products.**	Select option 7	Do not check option 7	________
		D	**Reaction stops during equilibrium.**	Check option 6 and do not check options 1 and 4	Do not check option 6 and check option 1 and / or 4	Do not check options 1, 4 and 6 / Check option 6 and option 1 and / or 4.
		E	**Reaction occurs during equilibrium, but only in one of the directions.**	Check only one of options 1 and 4 and do not check option 6.	Check options 1 and 4 and do not check option 6.	Do not check any of the options 1, 4 and 6. / Check option 6 alone.

1. Set of options II	Dynamic equilibrium/ reversibility	**F**	**Reactions in the forward and reverse directions do not occur simultaneously.**	Check at least one of the options 1 and 2	Do not check options 1 and 2.	______
		G	**Equilibrium may occur in a non-reversible reaction.**	Do not check option 3	Check option 3	______
1. Set of options III	Conditions for establishing equilibrium	**H**	**Difficulty in understanding equilibrium for almost complete reactions.**	Check option 1 or 3.	Do not check options 1 or 3	______
		I	**Incomprehension of the need for a closed system to establish the equilibrium in reactions with gas phase.**	Do not check option 2.	Check option 2.	______
2.	Quantitative composition of the equilibrium	**J**	**Confusion between equilibrium concentrations and stoichiometric coefficients.**	Check option C	Check option A or B	______
		K	**At equilibrium the total concentrations of products and reagents are the same.**	Check option A.	Check option B or C.	______
3.	Equilibrium disturbance by addition of reagents	**L**	**Misunderstanding of the meaning of adding a reagent.**	Concentration change of any species other than A and / or maintenance of the concentration of A	Increase in the concent. of A and maintenance of the concent. of the remaining species.	______
		M	**Misunderstanding that the reaction is moving in the forward direction as a response to the disturbance.**	Any combination except: higher concent. of products and lower concentration. of B. Independent of the concentrat. of A	Higher concent. of products and lower concentration. of B. Independent of the concentration of A.	______

		N	**The equilibrium moves in the forward direction, so in the new equilibrium state the concent. of the added reagent is less than or equal to its concentration in the first equilibrium.**	Higher concent. of products and lower concent. of B. Concent. of A less or equal.	Higher concent. of products and lower concentration. of B. Higher concent. of A.	Any other combination.
		O	**The value of the equilibrium constant can be altered by addition of reagent.**	Answer "yes" in question 3.4	Answer "no" in question 3.4	Blank or other answers.
4.	Equilibrium disturbance due to temperature change	**P**	**Incomprehension of the effect of temperature in the direction of equilibrium displacement**	Write greater or equal in the last space of 4.1 or true in option 1 of 4.2	Write smaller in the last space of 4.1 and false in option 1 of 4.2	———
		Q	**Incomprehension of the effect of temperature on the speed of the forward and reverse reactions.**	Any answer in 4.1 except: "greater" in the first two spaces.	Write larger in the first two spaces of 4.1	———
		R	**The value of the equilibrium constant cannot be changed by the temperature variation.**	True in option 2 of 4.2.	False in option 2 of 4.2	———
		S	**Changes in temperature do not cause changes in reagent and product concentrations.**	True in option 3 of 4.2	False in option 3 of 4.2	———
5.	Equilibrium disturbance due to pressure / volume change	**T**	**The decrease in volume is counteracted by the displacement of the equilibrium towards the formation of the largest number of gaseous moles.**	Answers that demonstrate agreement with the statement.	Disagreement with the statement. Indication of shift to the smallest number of gaseous moles.	Disagreement with the statement. No indication of shift to the smallest number of gaseous moles.
		U	**The addition of inert gas increases the pressure whereby the system moves towards the formation of the least number of gaseous moles (misunderstanding that the addition of inert gas does not affect equilibrium in ideal systems).**	Answers that demonstrate agreement with the statement.	Disagreement with the statement and indication that the addition of inert gas does not affect the equilibrium.	Disagreement with the statement without indicating that the addition of inert gas does not affect the equilibrium.

Stage I a) - Diagnosis of the difficulties in CE before the application of FACE approach (pre-test).

Table 6-3 Results from the pre-test.



Stage of Analysis I a
Dimension 1

Results
Pre-test Learning difficulties on CE

Student	**Categories**																				
	A	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**	**K**	**L**	**M**	**N**	**O**	**P**	**Q**	**R**	**S**	**T**	**U**
1	🟨	🟩	🟩	🟨	🟨	🟩	🟩	🟥	🟥	🟩	🟥	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟥	🟥	🟨
2	🟩	🟩	🟥	🟩	🟥	🟩	🟩	🟥	🟥	🟥	🟩	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟥	🟥	🟨
3	🟩	🟩	🟩	🟨	🟨	🟥	🟥	🟥	🟥	🟩	🟥	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟥	🟥	🟨
4	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟨	🟥	🟥	🟥	🟩	🟩	🟩	🟥
5	🟥	🟩	🟩	🟨	🟨	🟩	🟩	🟥	🟥	🟩	🟩	🟥	🟥	🟨	🟥	🟥	🟩	🟩	🟥	🟨	🟨
6	🟥	🟩	🟩	🟩	🟥	🟩	🟩	🟩	🟩	🟩	🟥	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟥	🟨	🟨
7	🟨	🟥	🟩	🟩	🟩	🟥	🟥	🟩	🟩	🟥	🟩	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟩	🟨	🟥
8	🟩	🟥	🟩	🟩	🟩	🟩	🟩	🟥	🟥	🟥	🟩	🟥	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟨	🟥
9	🟩	🟥	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟥
10	🟨	🟥	🟩	🟨	🟨	🟩	🟩	🟥	🟥	🟥	🟩	🟩	🟥	🟥	🟥	🟥	🟥	🟩	🟥	🟥	🟨
11	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟩	🟨	🟨
12	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟩	🟩	🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟩	🟩	🟩	🟨
13	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟩	🟩	🟥	🟥	🟥	🟥	🟥	🟥	🟥	🟩	🟥	🟩	🟨
14	🟨	🟩	🟩	🟩	🟥	🟥	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟥	🟨	🟨
15	🟨	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟥	🟩	🟥	🟩	🟩	🟩	🟥
16	🟨	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟩	🟥	🟩	🟥	🟩	🟩	🟩	🟥
17	🟩	🟩	🟥	🟥	🟨	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟥	🟥	🟩	🟥	🟩	🟩	🟩	🟥
18	🟥	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟥	🟥	🟩	🟥	🟩	🟥
19	🟩	🟩	🟩	🟨	🟨	🟩	🟩	🟥	🟥	🟥	🟩	🟥	🟥	🟩	🟥	🟥	🟥	🟩	🟥	🟥	🟥
20	🟩	🟩	🟩	🟨	🟨	🟥	🟥	🟥	🟥	🟥	🟩	🟥	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟥
21	🟥	🟩	🟩	🟩	🟥	🟥	🟥	🟩	🟩	🟥	🟩	🟥	🟩	🟥	🟩	🟥	🟥	🟩	🟥	🟩	🟥
22	🟥	🟩	🟩	🟩	🟥	🟥	🟥	🟩	🟩	🟥	🟩	🟥	🟩	🟥	🟩	🟥	🟥	🟩	🟩	🟩	🟥
23	🟥	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟩	🟥	🟥	🟥
24	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟩	🟥	🟥	🟥
25	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟥

🟥 Difficulty present
🟨 Inconclusive
🟩 Difficulty absence

Dimension of Analysis 1 - Learning Difficulties in CE **Data collection instrument: Post-test**

Table 6-4 Post-test pre-analysis: definition of categories and identification of indicators for the dimension of analysis 1.

Question	**Unity** (Topic under study)	**Category** (Difficulty / misconception to be detected)		Indicator of the presence of the category (the student manifests the difficulty)	Indicator of the absence of the category (The student does not manifests the difficulty)	Inconclusive answer
1. Set of options I	Chemical Equilibrium state	**A**	**The concentration of reagents and / or products changes during equilibrium state.**	Check option 1 and do not check option 2	Check option 2 and do not check option 1	Check options 1 and 2 or do not check any of these options.
		B	**The reaction rate decreases in equilibrium state**	Check option 4	Do not check option 4	————
		C	**Starting from the reactants a different equilibrium state is obtained, than starting from the products.**	Check option 5	Do not check option 5	————
		D	**Reaction stops during equilibrium.**	Check option 6 and do not check options 3 and 7.	Do not check option 6 and check option 3 and / or 7	Do not check options 3, 6 and 7 / Check option 6 and option 3 and / or 7.
		E	**Reaction occurs during equilibrium, but only in one of the directions.**	Check only one of options 3 and 7 and do not check option 6.	Check options 3 and 7 and do not check option 6.	Do not check options 3, 6 and 7. / Check option 6.
1. Set of options II	Dynamic equilibrium/ reversibility	**F**	**Reactions in the forward and reverse directions do not occur simultaneously.**	Check at least one of the options 1 and 3	Do not check options 1 and 3.	———
		G	**Equilibrium may occur in a non-reversible reaction.**	Do not check option 2	Check option 2	———

1. Set of options III	Conditions for establishing equilibrium	**H**	**Difficulty in understanding equilibrium for almost complete reactions.**	Check option 1 or 2.	Do not check options 1 or 2.	______
		I	**Incomprehension of the need for a closed system to establish the equilibrium in reactions with gas phase.**	Do not check option 3.	Check option 3.	______
2.	Quantitative composition of the equilibrium	**J**	**Confusion between equilibrium concentrations and stoichiometric coefficients.**	Check option C.	Check option A or B	______
		K	**At equilibrium the total concentrations of products and reagents are the same.**	Check option B.	Check option A or C.	______
3.	Equilibrium disturbance by addition of reagents	**L**	**Misunderstanding of the meaning of adding a reagent.**	Concentration change of any species other than B and / or maintenance of the concentration of B	Increase in the concent. of B and maintenance of the concent. of the remaining species.	______
		M	**Misunderstanding that the reaction is moving in the forward direction as a response to the disturbance.**	Any combination except: higher concent. of products and lower concentration. of A. Independent of the concentrat. of B.	Higher concent. of products and lower concentration. of A. Independent of the concentration of B.	______

		N	**The equilibrium moves in the forward direction, so in the new equilibrium state the concent. of the added reagent is less than or equal to its concentration. in the first equilibrium.**	Higher concent. of products and lower concentration of A. Concent. of B less or equal.	Higher concent. of products and lower concentration. of B. Higher concent. of A.	Any other combination.
		O	**The value of the equilibrium constant can be altered by addition of reagent.**	Answer "yes" in question 3.4	Answer "no" in question 3.4	Blank answer or other answers.
4.	Equilibrium disturbance due to temperature change	**P**	**Incomprehension of the effect of temperature in the direction of equilibrium displacement**	Write greater or equal in the last space of 4.1 or true in option 1 of 4.2	Write smaller in the last space of 4.1 and false in option 1 of 4.2	———
		Q	**Incomprehension of the effect of temperature on the speed of the forward and reverse reactions.**	Any answer in 4.1 except: “greater” in the first two spaces.	Write larger in the first two spaces of 4.1	———
		R	**The value of the equilibrium constant cannot be changed by the temperature variation.**	True in option 1 of 4.2	False in option 1 of 4.2	———
		S	**Changes in temperature do not cause changes in reagent and product concentrations.**	True in option 3 of 4.2	False in option 3 of 4.2	———
5.	Equilibrium disturbance due to pressure / volume change	**T**	**The decrease in volume is counteracted by the displacement of the equilibrium towards the formation of the largest number of gaseous moles.**	Answers that demonstrate agreement with the statement.	Disagreement with the statement. Indication of shift to the smallest number of gaseous moles.	Disagreement with the statement. No indication of shift to the smallest number of gaseous moles.
		U	**The addition of inert gas increases the pressure whereby the system moves towards the formation of the least number of gaseous moles (misunderstanding that the addition of inert gas does not affect equilibrium in ideal systems).**	Answers that demonstrate agreement with the statement.	Disagreement with the statement and indication that the addition of inert gas does not affect the equilibrium.	Disagreement with the statement without indicating that the addition of inert gas does not affect the equilibrium.

Stage I b) - Diagnosis of the difficulties in CE after the application of FACE approach (post-test).

Table 6-5 Results from the post-test.

Stage of Analysis I b. **Results**
Dimension 1 **Post-test Learning difficulties on CE**

Student	**Categories**																				
	A	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**	**K**	**L**	**M**	**N**	**O**	**P**	**Q**	**R**	**S**	**T**	**U**
1	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟥	🟥	🟥	🟩	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟥	🟥	🟨
2	🟨	🟩	🟩	🟩	🟥	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟩	🟩	🟥	🟥	🟩
3	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟥	🟥	🟥	🟩	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟥	🟥	🟨
4	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟩
5	🟩	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟩	🟩	🟥	🟨	🟩
6	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟩	🟩	🟥	🟥	🟩
7	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟥	🟩	🟩	🟥	🟩	🟥	🟩	🟥
8	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟥	🟩	🟩	🟥	🟩	🟩	🟨	🟥
9	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟩
10	🟨	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟥	🟥	🟩	🟥	🟥	🟩	🟩	🟩	🟥	🟩	🟥	🟨	🟨
11	🟩	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟨	🟨
12	🟩	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟨
13	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟨
14	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟨	🟥	🟥	🟥	🟩	🟩	🟨	🟨
15	🟨	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟥	🟩	🟩	🟨	🟥
16	🟨	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟥	🟩	🟩	🟨	🟥
17	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟥	🟥	🟥	🟩	🟥	🟩	🟩
18	🟥	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟥	🟥	🟥	🟩	🟥	🟩	🟩
19	🟥	🟩	🟩	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟥	🟥	🟩	🟥	🟥	🟥
20	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟥	🟩	🟥	🟥	🟩	🟩	🟩	🟨
21	🟥	🟩	🟩	🟩	🟩	🟥	🟥	🟩	🟩	🟥	🟩	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟥
22	🟥	🟩	🟩	🟩	🟩	🟥	🟥	🟩	🟩	🟥	🟩	🟩	🟥	🟨	🟩	🟥	🟥	🟩	🟩	🟩	🟥
23	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟥	🟩	🟩	🟥	🟨	🟩	🟥	🟩	🟩	🟥	🟨	🟨
24	🟥	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟩	🟩	🟥	🟥	🟩	🟩	🟩	🟥
25	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩	🟥	🟩	🟩	🟩	🟥	🟩	🟩	🟨	🟨

🟥 Difficulty present
🟨 Inconclusive
🟩 Difficulty absence

Table 6-6 Exploration guide pre-analysis: definition of categories and identification of indicators for the analysis.

Category		Action related on the exploration guide	Correct Answer	Wrong answer
A	**The concentration of reagents and / or products changes during equilibrium state.**	First question on the reflection from activity 1.	Yes	No
B	**The reaction rate decreases in equilibrium state.**	Third question on the reflection from activity 1.	No	Yes
C	**Starting from the reactants a different equilibrium state is obtained, than starting from the products.**	Activity 4 from the exploration guide.	Registration of equal values and concluding that there is no difference.	Other answers
D	**Reaction stops during equilibrium.**	Second question on the reflection from activity 1.	No	Yes
E	**Reaction occurs during equilibrium, but only in one of the directions.**	Actions from activity 1	--------	--------
F	**Reactions in the forward and reverse directions do not occur simultaneously.**	Actions from activity 1	--------	______
G	**Equilibrium may occur in a non-reversible reaction.**	No specific actions on the exploration guide.	------	______
H	**Difficulty in understanding equilibrium for almost complete reactions.**	No specific actions on the exploration guide.		______
I	**Incomprehension of the need for a closed system to establish the equilibrium in reactions with gas phase.**	No specific actions on the exploration guide.		______
J	**Confusion between equilibrium concentrations and stoichiometric coefficients.**	Quantities registered in activities 2, 4 and 5.	Registration of values retrieved the simulation.	Registering deliberately stoichiometric values from the equation.
K	**At equilibrium the total concentrations of products and reagents are the same.**	Fourth question on the reflection from activity 1	No	Yes/other
L	**Misunderstanding of the meaning of adding a reagent.**	Conclusions from activity 5	Systems shifts in the forward direction.	Other answers
M	**Misunderstanding that the reaction is moving in the forward direction as a response to the disturbance.**	Activity 5, answer to: “Direction of equilibrium displacement”.	Forward	Reverse or other answers

Category		Action related on the exploration guide	Correct Answer	Wrong answer
N	**The equilibrium moves in the forward direction, so in the new equilibrium state the concent. of the added reagent is less than or equal to its concentration. in the first equilibrium.**	Registering quantities of reactants in activity 5 and reflection.	Registration of correct values from the simulation, acknowledging the increase in quantities.	Other answers
O	**The value of the equilibrium constant can be altered by addition of reagent.**	Registering equilibrium constants in activity 5 and reflection.	Registering equilibrium constants correctly in activity 5 and reflection.	Other answers
P	**Incomprehension of the effect of temperature in the direction of equilibrium displacement.**	Registrations from activity 2	Refer that a higher temperature corresponds to a shift in the reverse direction and selecting exothermic.	Other answers
Q	**Incomprehension of the effect of temperature on the speed of the forward and reverse reactions.**	Reflection from activity 2	Raising temperature speeds up the reactions but not necessarily the reactions extension.	Other combinations of answers.
R	**The value of the equilibrium constant cannot be changed by the temperature variation.**	Registration of equilibrium constants in activity 2	Registration of correct (different) equilibrium constants in the 1st and 2nd equilibriums.	Registration of wrong equilibrium constants in the 1st and 2nd equilibriums.
S	**Changes in temperature do not cause changes in reagent and product concentrations.**	Registration of quantity of products in activity 2	Registration of correct (different) quantities of products in the 1st and 2nd equilibriums.	Registration of wrong (different or otherwise) quantities of products in the 1st and 2nd equilibriums
T	**The decrease in volume is counteracted by the displacement of the equilibrium towards the formation of the largest number of gaseous moles.**	Reflection from activity 3	Correctly applying Le Chatelier's principle to pressure.	Misapplying Le Chatelier's Principle
U	**The addition of inert gas increases the pressure whereby the system moves towards the formation of the least number of gaseous moles (misunderstanding that the addition of inert gas does not affect equilibrium in ideal systems).**	Registrations and conclusions from activity 6	Answering: • No shift on an ideal system • Reverse in a real system • Concluding accordingly	Any other combination of answers

Stage I c)- Diagnosis of the CE knowledge during the application of FACEapproach (exploration guide).

Table 6-7 Results from the exploration guide.

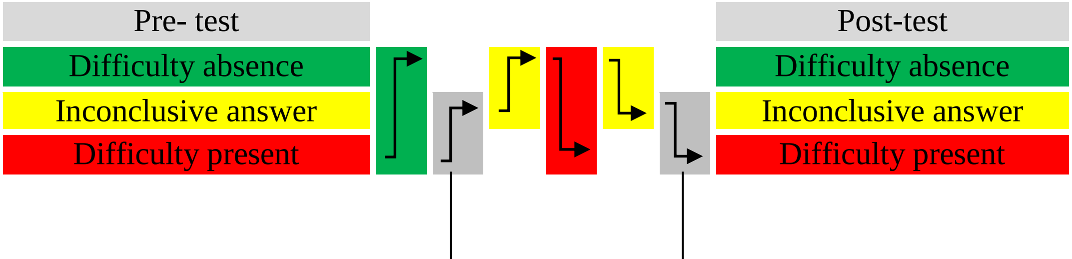
Category	correct answers frequency	no answers frequency	wrong answers frequency	percentage of correct answers	Notes
A	23	0	2	92%	
B	22	0	3	88%	
C	20	1	4	80%	
D	25	0	0	100,0%	
E	----	----	----	----	
F	----	----	----	----	
G	----	----	----	----	
H	----	----	----	----	
I	----	----	----	----	
J	25	0	0	100,0%	
K	24	0	1	96%	
L	9	9	7	36%	Several students indicated in the conclusion a shift in the direction with smaller number of moles.
M	22	3	0	88%	
N	21	3	1	84%	
O	20	3	2	80%	
P	20	0	5	80%	Students who started with higher temperature and then lower temperature tended to fail
Q	20	0	5	80%	
R	25	0	0	100,0%	
S	21	0	4	84%	
T	8	0	17	32%	
U	6	3	16	24%	Several students reached the right conclusion but answered shift in the forward direction for an ideal system

6.5.2. Stage II – Comparative analysis (improvements / setbacks) in learning

In stage two we focus on comparing the results obtained in the pre-test and the post-test for each category. Since this study has a qualitative character, the counts we make in this stage have the purpose of serving as a base for further analysis in future stages, where data from several instruments is triangulated and descriptive information about FACE approach is traced.

In order to compare post-test and pre-test results we have studied the movements students could make in each category:

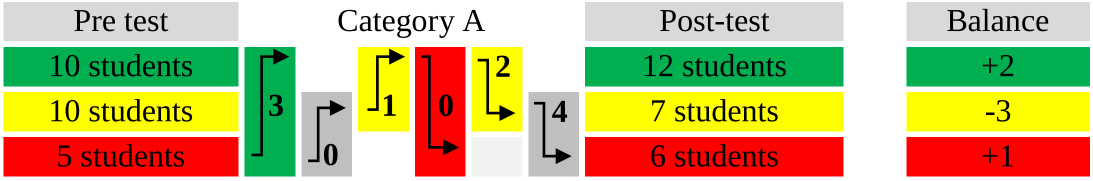
Possible student movements between pre-test and post-test



Pre- test	Post-test
Difficulty absence	Difficulty absence
Inconclusive answer	Inconclusive answer
Difficulty present	Difficulty present

Non-significant movements: it is not considered an improvement or setback the passage from the presence of difficulty to an inconclusive answer or the opposite.

Example:



Pre test	Category A	Post-test	Balance
10 students		12 students	+2
10 students		7 students	-3
5 students		6 students	+1

The balance of the “difficulty absences” is an important parameter, since it reflects all significant movements performed by the students globally. So, we have calculated the percentage of students who have improved dividing the balance of difficulty absences by the number of students that could improve (frequency of pre-test presence and inconclusive indicators). Nevertheless, the balance values do not translate individual movements of the students. In “red” balance for instance, we only get to know the quantity of students that had a difficulty in the end minus the number of students that had the same difficulty in the beginning. So we have considered other parameters, like the percentage of positive movements. This parameter tells us how many students have improved in the universe of all the students that revealed movements from the pre-test to the post-test. Positive movements (upward) include moving from the presence of the difficulty to the absence or from an inconclusive answer to the absence of the difficulty. Table 6.8 summarizes this analysis and Table 6.9 illustrates the movements in the style from Tables 6.3 and 6.5.

Table 6-8 Results of the comparative analysis of the pre-test / post-test - Learning difficulties in CE

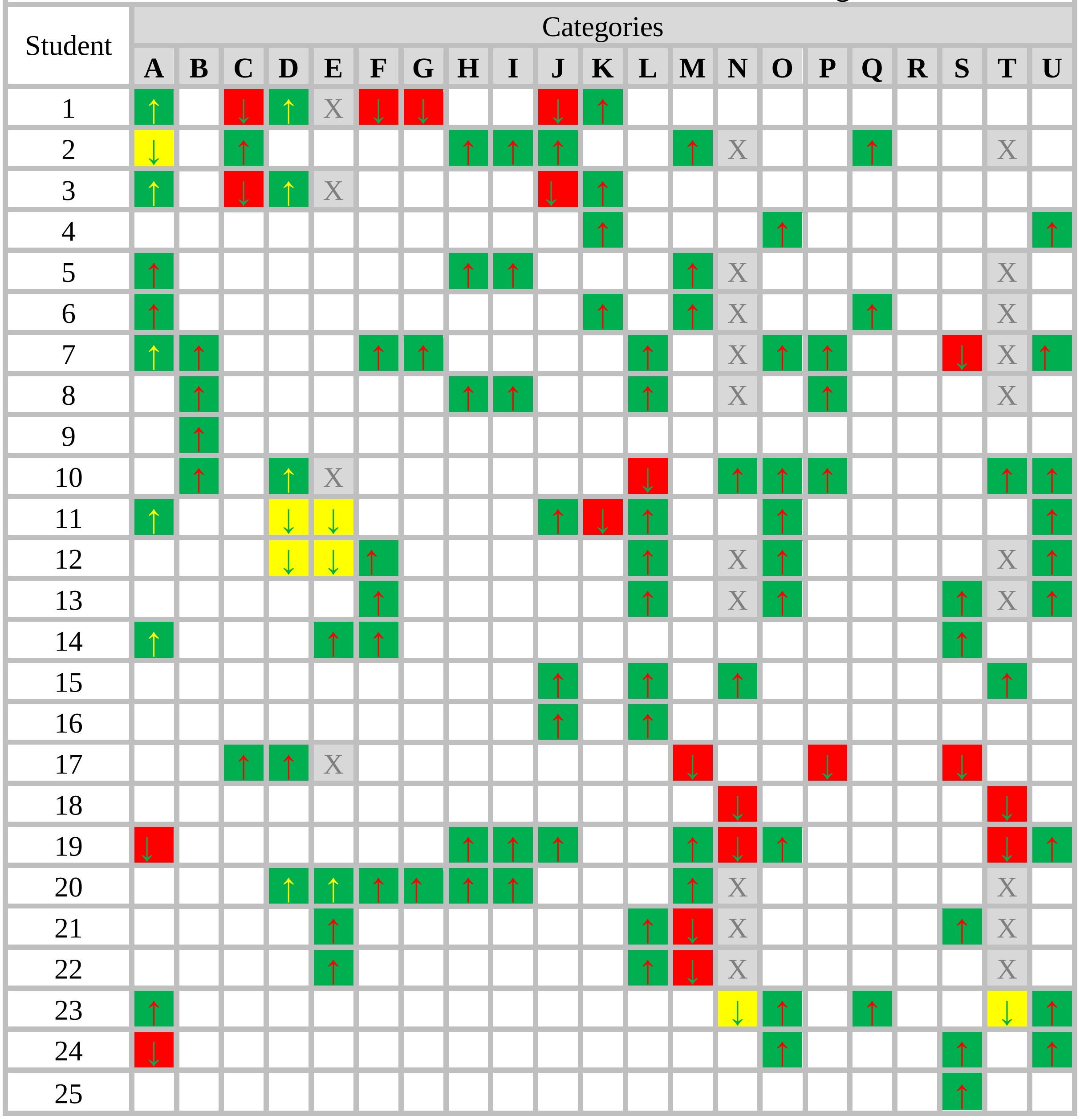
Stage of Analysis II
Dimension of Analysis 1 **Comparative analysis Pre-test / Post-test - Learning difficulties in CE**

	Parameter	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
Frequency of the difficulty in the sample	Pre-test Presences | Inconc. | Absences	6 8 11	4 21	2 23	1 9 15	5 10 10	8 17	5 20	9 16	8 17	17 8	6 19	19 6	21 4	7 12 6	19 0 6	21 4	24 1	0 25	14 11	7 6 12	15 10 0
	Post-test Presences | Inconc. | Absences	5 4 16	0 25	2 23	0 7 18	6 7 12	4 21	4 21	4 21	3 22	14 11	3 22	11 14	19 6	9 11 5	10 0 15	19 6	21 4	0 25	11 14	5 9 11	8 10 7
	Balance post-test/ pre-test Presences | Inconc. | Absences	-1 -4 +5	-4 +4	0 0	-1 -2 +3	+1 -3 +2	-4 +4	-1 +1	-5 +5	-5 +5	-3 +3	-3 +3	-8 +8	-2 +2	+2 -1 -1	-9 0 +9	-2 +2	-3 +3	0 0	-3 +3	-2 +3 -1	-7 0 +7
	Percentage of students who have improved*	36%	100%	0%	30%	13%	50%	20%	56%	63%	18%	50%	42%	10%	-5%	47%	10%	13 %	-	21%	-8%	28%
Movements of the students between pre-test and post-test	Presence → Absence	3	4	2	1	3	5	2	5	5	5	4	9	5	2	9	3	3	-	5	2	7
	Inconc. → Absence	5	-	-	4	1	-	-	-	-	-	-	-	-	0	0	-	-	-	-	0	0
	Absence → Inconc.	1	-	-	2	2	-	-	-	-	-	-	-	-	1	0	-	-	-	-	1	0
	Absence → Presence	2	0	2	0	0	1	1	0	0	2	1	1	3	2	0	1	0	0	2	2	0
	Non-significant movements (Presences⇔ Inconc.)	0	-	-	0	4	-	-	-	-	-	-	-	-	10	0	-	-	-	-	10	0
	Percentage of favourable significant movements**	8/11 73%	4/4 100%	2/4 50 %	5/7 71%	4/6 67%	5/6 83%	2/3 67%	5/5 100%	5/5 100%	5/7 71%	4/5 80%	9/10 90%	5/8 63%	2/5 40%	9/9 100%	3/4 75%	3/3 100%	0	5/7 71%	2/5 40%	7/7 100%

*Calculated from: balance of absences /students that could improve (frequency of pre-test presences and inconclusive)

**Calculated from: summation of positive movements / summation of all significant movements

Stage of Analysis II **Dimension of Analysis 1**
Movements between Pre-Test and Post-test **Learning difficulties in CE**



Student	Categories																				
	A	**B**	**C**	**D**	**E**	**F**	**G**	**H**	**I**	**J**	**K**	**L**	**M**	**N**	**O**	**P**	**Q**	**R**	**S**	**T**	**U**
1	🟩↑		🟥↓	🟩↑	X	🟥↓	🟥↓			🟥↓	🟩↑										
2	🟨↓		🟩↑					🟩↑	🟩↑	🟩↑			🟩↑	X			🟩↑			X	
3	🟩↑		🟥↓	🟩↑	X					🟥↓	🟩↑										
4											🟩↑				🟩↑						🟩↑
5	🟩↑							🟩↑	🟩↑				🟩↑	X						X	
6	🟩↑										🟩↑		🟩↑	X			🟩↑			X	
7	🟩↑	🟩↑				🟩↑	🟩↑					🟩↑		X	🟩↑	🟩↑			🟥↓	X	🟩↑
8		🟩↑						🟩↑	🟩↑			🟩↑		X		🟩↑				X	
9		🟩↑																			
10		🟩↑		🟩↑	X							🟥↓		🟩↑	🟩↑	🟩↑				🟩↑	🟩↑
11	🟩↑			🟨↓	🟨↓					🟩↑	🟥↓	🟩↑			🟩↑						🟩↑
12				🟨↓	🟨↓	🟩↑						🟩↑		X	🟩↑					X	🟩↑
13						🟩↑						🟩↑		X	🟩↑				🟩↑	X	🟩↑
14	🟩↑				🟩↑	🟩↑													🟩↑		
15										🟩↑		🟩↑		🟩↑						🟩↑	
16										🟩↑		🟩↑									
17			🟩↑	🟩↑	X								🟥↓			🟥↓			🟥↓		
18														🟥↓						🟥↓	
19	🟥↓							🟩↑	🟩↑	🟩↑			🟩↑	🟥↓	🟩↑					🟥↓	🟩↑
20				🟩↑	🟩↑	🟩↑	🟩↑	🟩↑	🟩↑				🟩↑	X						X	
21					🟩↑							🟩↑	🟥↓	X					🟩↑	X	
22					🟩↑							🟩↑	🟥↓	X						X	
23	🟩↑													🟨↓	🟩↑		🟩↑			🟨↓	🟩↑
24	🟥↓														🟩↑				🟩↑		🟩↑
25																			🟩↑		

Table 6-9 Results from the post-test.

🟩↑	Presence of learning difficulty (pre-test) → absence of difficulty (post-test)
🟩↑	Inconclusive answer (pre-test)→ absence of learning difficulty (post-test).
🟨↓	Absence of learning difficulty (pre-test) → inconclusive answer (post-test).
🟥↓	Absence of learning difficulty (pre-test) → presence of difficulty (post-test).
X	Non-significant movements: Inconclusive response (pre-test) ←→ presence of learning difficulty (post-test).

To finish stage of analysis II, we present Table 6.10 which purpose is to expose the difficulties and misconceptions that were present in larger number in our student sample, as well as identifying the categories with noticeable improvements after the use of FACE approach.

Table 6-10 Difficulties and misconceptions distribution in the sample.

Difficulties not present in the sample both in the pre-test and post-test.	**R**	**The value of the equilibrium constant cannot be changed by the temperature variation.**
Difficulties present in more than 20 students in the pre-test.	**M** **P** **Q**	**Misunderstanding that the reaction is moving in the forward direction as a response to the disturbance.** **Incomprehension of the effect of temperature in the direction of equilibrium displacement.** **Incomprehension of the effect of temperature on the speed of the forward and reverse reactions.**
Difficulties present in more than 20 students in the post-test.	**Q**	**Incomprehension of the effect of temperature on the speed of the forward and reverse reactions.**
Difficulties present in 16 to 20 students in the pre-test.	**J** **L** **O**	**Confusion between equilibrium concentrations and stoichiometric coefficients.** **Misunderstanding of the meaning of adding a reagent.** **The value of the equilibrium constant can be altered by addition of reagent.**
Difficulties present in 16 to 20 students in the post-test.	**M** **P**	**Misunderstanding that the reaction is moving in the forward direction as a response to the disturbance.** **Incomprehension of the effect of temperature in the direction of equilibrium displacement.**
Difficulties with percentage of improvement equal or superior to 50%.	**B** **F** **H** **I** **K**	**The reaction rate decreases in equilibrium state.** **Reactions in the forward and reverse directions do not occur simultaneously.** **Difficulty in understanding equilibrium for almost complete reactions.** **Incomprehension of the need for a closed system to establish the equilibrium in reactions with gas phase.** **At equilibrium the total concentrations of products and reagents are the same.**
Difficulties without improvement or with a setback.	**C** **N** **T**	**Starting from the reactants a different equilibrium state is obtained, than starting from the products.** **The equilibrium moves in the forward direction, so in the new equilibrium state the concent. of the added reagent is less than or equal to its concentration. in the first equilibrium.** **The decrease in volume is counteracted by the displacement of the equilibrium towards the formation of the largest number of gaseous moles.**

6.5.3. Stage III - Collection of indicators about familiarization with CE language and participation/interest revealed by the students.

Progressing to dimension of analysis 2 we have searched in the tests and the exploration guide for indicators related to the “familiarization with equilibrium language”, gathering the information presented in table 6.11. In what concerns to this dimension of analysis the indicators were defined by performing a transversal reading of the content of the tests and the exploration guides. Only the open questions of the tests were included in this analysis. Also, in the exploration guide we have used content from the reflections and conclusions proposed to the students in each activity.

Some notes about dimension of analysis 2:

- In the pre-test several students refer Le Chatelier’s principle, but without expanding on it, just referring that the question is related to this law.
- It is more common in the pre-test the referral to shifts in equilibrium in informal language such as “the reaction will form in the forward direction”, “the reaction will react” or “the reaction will change.”
- In the post-test several students answered “the same as in questionnaire A”, not answering directly to the question posed and thus not providing any data except for their participation and interest.

Table 6-11 Results from dimension of analysis 2 – Familiarization with equilibrium language.

Dimension of analysis 2 – Familiarization with equilibrium language					
Category	**Indicators**	**Pre-test freq.**	**Post-test freq.**	**Exp. Guide freq.**	**Examples**
Le Chatelier´s principle and equilibrium disturbances	The system counteracts according to Le Chatelier´s principle.	16	2	0	*"This question is about Le Chatelier's law(…)"*
	Pressure relation to the number of gaseous moles.	8	7	11	*"Increasing the pressure the reaction shifts in the direction with smaller number of gaseous moles."*
	Temperature's relation to the extension of the reaction.	0	0	3	*"In an exothermic reaction, when raising the temperature, K value decreases."*
	The reaction is favoured/evolving in the forward/reverse direction.	8	8	10	*"The addition of reactant favours the forward direction."*
Reversibility and Equilibrium	References to forward and inverse reactions.	8	7	16	*"The reaction will spend reactant so it will evolve in the forward direction."*
	References to shift in equilibrium/system.	4	6	0	*"If we add reagents to the reaction this will tend to shift in the forward direction."*
	Direct references to reversibility.	0	2	0	*"Since the reaction is reversible, both products and reactants form simultaneously."*
Yield and productivity	References to the extension of the reaction and productivity.	0	0	2	*"I took these options because I gave attention to the extension of the reaction that was higher, and so, the productivity rose, as well as profits."*
Kinetics and equilibrium	Greater velocity does not mean greater extension.	0	0	5	*"No, in this reaction, higher velocity corresponds to smaller product concentrations."*

Now, in order to cross information from the different sources of data collection we have to consider also the observation and notes registered by the investigator along the case study. This information will be relevant for all the dimensions of analysis but specially to dimension 3 - Participation and interest of the students. Table 6.12 presents the most relevant notes from the observation process.

Table 6-12 Observation /notes.

Observation / Notes			
Students opinions /interventions	*Completing the exploration guide*	*Students interaction with FACE approach*	
"…it allowed us to deepen our knowledge."	*Students next to each other have similar answers.* *Some students leave in blank the questions, especially in the activities close to the end of the exploration guide.* *Open answers, conclusion and reflections also have been left blank by a considerable number of students, either in the tests or the exploration guide.*	*Some dispersion of the students during the exploration of the simulation: they first tried everything, including the achievement of the most economically favourable process. Only after that did they start reading the exploration guide.* *Students were interested in exploring the simulation (especially in observing submicro representation and the productivity obtained) and happy to have the opportunity of using an interactive resource during the lesson.* *Students perform the actions proposed in the exploration guide without revealing difficulties or asking for much help.* *Students seem to get more familiar with equilibrium language along the activity.*	*Students benefit from discussing among themselves during the exploration of the simulation.*
"So, this is how it works!" (expression made by one of the students, when answering a question in the post-test after having explored the simulation).			*Importance of a final dialogue with the students to point out conclusions, since it seems to be too much information for students to acquire in 90 minutes.* *Teacher's role appears to be determinant in the success of the approach, namely accompanying the students and promote/guide the reflections and conclusions.*

In what concerns to the third dimension of analysis – participation/ interest revealed by the students, several indicators point that students were motivated with the activity, like the investigator noticing a good level of interaction with the simulation. Also, students' opinions and behaviour point that they found pedagogical relevance in FACE approach. Nevertheless, the participation of the students in the exploration guide, namely blank answers constitute negative indicators. Table 6.13 reunites the positive and negative indicators concerning dimension of analysis 3 – Participation/ Interest revealed by the students.

Table 6-13 Results from dimension of analysis 3 – Participation/ Interest revealed by the students.

Dimension of analysis 3 – Participation/ Interest revealed by the students	
Positive indictors	**Negative indicators**
• **Students interaction with the simulation and the teacher;** • **Collaboration between the students who share a computer;** • **Usability of the simulation and easy understanding of the actions proposed in the exploration guide;** • **Students' opinions referring the interest and pedagogical relevance of the simulation.**	• **Several questions left blank in the exploration guide, especially in the activities close to the end;** • **Some indifference to the relevance of the post-test;** • **Some lack of persistence of the students in reflecting and concluding in order to consolidate knowledge acquired by exploring the simulation.**

6.5.4. Stage IV- Cross-reference and interpretation of data in order to relate the results with the content of FACE approach

In the last stage from data analysis we use the results from the three dimensions, in order to relate them with the content of FACE approach. By processing this last stage of analysis we intend to serialize the components/elements of the approach associated to a particular result. This study will allow discussing later the relevance of the theoretical assumptions made in the construction of FACE approach as well as tracing suggestions for its reformulation. Table 6.14 presents the analysis performed in stage IV.

Table 6-14 Stage of analysis IV

	Contribution from Dimension of Analysis 1				Contribution from Dimensions of analysis II and III	Crossing the results with FACE approach content	
	Categories	Pre-test post-test comparative analysis	Exploration guide analysis	Notes		Simulation Elements related	Response of FACE approach
		🟥 ≤ 50% 🟨 🟩 > 75%	🟥 ≤ 50% 🟨 🟩 > 75%				
		Percentage of favourable significant movements	Percentage of correct answers				
A	**The concentration of reagents and / or products changes during equilibrium state.**	**73%**	**92%**	**------**	**------**	**Verify the maintenance of composition during equilibrium - Chemical equilibrium as a static macro event.**	**Face response was positive. The simulation directly shows the concentrations of equilibrium remaining constant and the exploration guide questions the student about this fact having the large majority answered correctly. Nevertheless, an even better result was expected in this category from pre-test to post-test.**
B	**The reaction rate decreases in equilibrium state.**	**100%**	**88%**	**This category was present only in four students from the sample. Nevertheless, 100% of the students improved in the post test**	**Students revealed positive interaction with the simulation, especially the submicro representation;**	**Dynamic equilibrium simulation through molecular movement.** **Simulating microscopically the evolution to equilibrium.**	**The permanence of the motion of the particles associated to the question that reflects upon this fact seems to provide very good results in avoiding the idea that the reaction rate decreases during equilibrium.**

Categories		Pre-test post-test comparative analysis	Exploration guide analysis	Notes	Contribution from Dimensions of analysis II and III	Simulation Elements related	Response of FACE approach
C	**Starting from the reactants a different equilibrium state is obtained, than starting from the products.**	**50%**	**80%**	**Only two students had the difficulty in the pre-test and although they have improved, two other students failed in the post-test.**	**Students appear to consider the exploration guide too big and too much information to retain in 90 minutes.**	**Quantitative values for the composition of the system during reaction progress and equilibrium.**	**Although one of the activities from the exploration guide is dedicated to this idea and the simulation clearly allows verifying that the same quantities are obtained, the results from the tests are not positive. Some answers to the exploration guide suggest that although students recognize that the same quantities are achieved, the industrial production will be different starting from products or reactants (could this have been the confusing factor?). Should the exploration guide be smaller to avoid blank answers by the end? Is it worth it to dedicate an entire activity to this category?**
D	**Reaction stops during equilibrium.**	**71%**	**100%**	-----	**Students revealed positive interaction with the simulation, especially the submicro representation;**	**Dynamic equilibrium simulation through molecular movement.**	**The continuation of the motion of the particles associated to the question that reflects upon this fact provides good results in the exploration guide although some resistance to this idea prevails in the post-test.**
E	**Reaction occurs during equilibrium, but only in one of the directions.**	**67%**	-----	**Exploration guide approaches this category in the actions proposed in the activities but no specific registrations or questions are associated.**		**Dynamic equilibrium simulation through molecular movement.** **Double arrow in chemical equations**	**Results but could be better, perhaps due to the lack of a short answer question concerning this idea in the exploration guide.**
F	**Reactions in the forward and reverse directions do not occur simultaneously.**	**83%**	-----		**Students revealed positive interaction with the simulation, especially the submicro representation;**	**Simulating microscopically the evolution to equilibrium.**	**The simulation of the microscopic constant movement, with “dot colour mixing”, appears to eliminate the idea of compartmentalised view of chemical equilibrium.**

Categories		Pre-test post-test comparative analysis	Exploration guide analysis	Notes	Contribution from Dimensions of analysis II and III	Simulation Elements related	Response of FACE approach
G	**Equilibrium may occur in a non-reversible reaction.**	**67%**	-----		**Students make direct references to reversibility in the post-test.**	**Verify a case of incomplete reaction (neither of the reactants is depleted).** **Possibility to start the reaction from reagents or products (macro idea of reversibility).** **Possibility to disturb equilibrium.**	**Actions in the simulation, especially disturbances allow students to consolidate the idea of reversibility as being connected to equilibrium reactions. Nevertheless, some students still fail in this category in the post-test.**
H	**Difficulty in understanding equilibrium for almost complete reactions.**	**100%**	----	**The exploration guide approaches this category in the actions proposed in the activities but no specific registrations or questions are associated.**	-----	**Quantitative values for the composition of the system.** **Equilibrium law (*K*) and associated calculations**	**The diversity of values and different equilibrium constants students observe and register along the approach appear to enlarge their view about the multiplicity of equilibrium states possible.**
I	**Incomprehension of the need for a closed system to establish the equilibrium in reactions with gas phase.**	**100%**	----		-----	**Closed reactor as a macroscopic analogy.**	**Actions in the simulation allow students to get familiar with a gaseous system in a closed reactor, where equilibrium is established.**
J	**Confusion between equilibrium concentrations and stoichiometric coefficients.**	**71%**	**100%**	**17 students revealed this difficulty in the pre-test.**	-----	**Quantitative values for the composition of the system during reaction progress and equilibrium.** **Reaction equation**	**Face approach has partially improved results in a category where several students revealed difficulties. Nevertheless, although students register correct values in the exploration guide, this activity does not seem to create sufficient conflict to promote conceptual change in most of the students that reveal the difficulty, reason why several students still fail in post-test question about this category.**

Categories		Pre-test post-test comparative analysis	Exploration guide analysis	Notes	Contribution from Dimensions of analysis II and III	Simulation Elements related	Response of FACE approach
K	**At equilibrium the total concentrations of products and reagents are the same.**	**80%**	**96%**	------	------	**Quantitative values for the composition of the system during reaction progress and equilibrium**	**Face approach has considerably improved results.**
L	**Misunderstanding of the meaning of adding a reagent.**	**90%**	**36%**	**19 students revealed this difficulty in the pre-test. The Exploration guide's bad results are explained by the fact that although students correctly register the direction of equilibrium shift they tend to associate it with smaller number of gaseous moles.**	**Pressure's relation to the number of gaseous moles is the most frequent indicator related to the familiarization with equilibrium language.**	**Possibility to disturb equilibrium (addition of reagent).** **Le Chatelier´s principle application – prediction of effects.**	**Students recognize that system displacement is in the forward direction when adding a reactant, which justifies the good results in the post-test. Nevertheless, in the exploration guide several students include the information that the system shifts in the direction of the smaller number of gaseous moles, confusing this disturbance with changes in pressure. Pressure changes are worked upon in a previous activity in the exploration guide, which has certainly contributed to the confusion. Also students reveal to be very familiar with the language referring to changes in pressure.**
M	**Misunderstanding that the reaction is moving in the forward direction as a response to the disturbance.**	**63%**	**88%**	----	**There is not much difference in the frequency that students use terms related to shifts in equilibrium from pre-test to post-test.**	**Le Chatelier´s principle application.** **Visualization of Q gradual approximation to K** **Underlined arrow showing equilibrium shift**	**Most students answer correctly to the exploration guide but, again, exploring the simulation and answering as expected to the exploration guide seems to be insufficient to destroy misconceptions in several students.**

Categories		Pre-test post-test comparative analysis	Exploration guide analysis	Notes	Contribution from Dimensions of analysis II and III	Simulation Elements related	Response of FACE approach
N	**The equilibrium moves in the forward direction, so in the new equilibrium state the concent. of the added reagent is less than or equal to its concentration. in the first equilibrium.**	**40%**	**84%**	----	**The frequency of indicators in the pre-test shows that students were already very familiar with Le Chatelier´s principle typical enunciation but not so good in applying it.**	**Quantitative values for the composition of the system during reaction progress and equilibrium**	**Typical situation where students answer correctly to the exploration guide and register the conclusion proving that they notice that the quantity of reagent is superior in second equilibrium. Nevertheless, they fail to answer correctly in the post –test. This specific case appears to be related to the use of Le Chatelier's principle typical language.**
O	**The value of the equilibrium constant can be altered by addition of reagent.**	**100%**	**80%**	**19 students revealed this difficulty in the pre-test.**	-----	**Quantitative analysis of equilibrium displacements using Q and K values.** **Equilibrium law (K) and associated calculations**	**Face approach provide good results in a category present in several students**

Categories		Pre-test post-test comparative analysis	Exploration guide analysis	Notes	Contribution from Dimensions of analysis II and III	Simulation Elements related	Response of FACE approach
P	Incomprehension of the effect of temperature in the direction of equilibrium displacement.	75%	80%	21 students revealed this difficulty in the pre-test.	Seems to be too much information for students to acquire in 90 minutes.	Information about reaction enthalpy. Equilibrium law (K) and associated calculations. Quantitative values for the composition of the system. Quantitative analysis of equilibrium displacements using Q and K values. Le Chatelier´s principle application – prediction of effects. Possibility to disturb equilibrium.	Face approach has partially improved results in categories where a large number of students revealed difficulties. The fact that several elements of the simulation have to be crossed in this category can justify the difficulties. Students must consider kinetics, equilibrium law, enthalpy, system composition and Le Chatelier´s principle in order to deal with all the aspects from temperature disturbances. This can clearly overload memory working space and implies abstracting over previous abstractions.
Q	Incomprehension of the effect of temperature on the speed of the forward and reverse reactions.	100%	80%	24 students revealed this difficulty in the pre-test. Although all the movements were positive, only 3 students have improved.	-----	Dynamic equilibrium simulation through molecular movement. Simulating microscopically the evolution to equilibrium.	
R	The value of the equilibrium constant cannot be changed by the temperature variation.	No students reveal the difficulty in the pre-test or post-test.	100%	-----	-----	Equilibrium law (K) and associated calculations Visualization of Q gradual approximation to K Possibility to disturb equilibrium.	Students from the sample had already acquired the idea that K changes with the temperature.

Categories		Pre-test post-test comparative analysis	Exploration guide analysis	Notes	Contribution from Dimensions of analysis II and III	Simulation Elements related	Response of FACE approach
S	**Changes in temperature do not cause changes in reagent and product concentrations.**	**71%**	**84%**	**----**	**----**	**Quantitative values for the composition of the system.** **Possibility to disturb equilibrium.**	**Face approach has partially improved results.**
T	**The decrease in volume is counteracted by the displacement of the equilibrium towards the formation of the largest number of gaseous moles.**	**40%**	**32%**	**----**	**The frequency of indicators in the pre-test shows that students were already very familiar with Le Chatelier´s principle typical enunciation but not so good in applying it.**	**Quantitative analysis of equilibrium displacements using Q and K values.** **Visualization of Q gradual approximation to K** **Possibility to disturb equilibrium.**	**Students continue to apply Le Chatelier's principle to volume variations even after FACE approach, one of the categories with the worst response.**
U	**The addition of inert gas increases the pressure whereby the system moves towards the formation of the least number of gaseous moles (misunderstanding that the addition of inert gas does not affect equilibrium in ideal systems).**	**100%**	**24%**	**All students registered difficulties or inconclusive answers in the pre-test. Several students reached the right conclusion but answered shift in the forward direction for an ideal system.**	**Students lack of persistence in answering the questions from the last activities in the exploration guide.**	**Quantitative analysis of equilibrium displacements using Q and K values.** **Quantitative values for the composition of the system.** **Effect of the addition of inert gas to equilibrium**	**For this category it seems that the activity from the exploration guide caused some misunderstanding in the students, since they were able to improve in the post-test but registered wrong data in the exploration guide.**

6.6. Discussion of results

The analysis of the results presented in the previous section leads us to conclude that, in general, FACE approach contains components with potential to reduce the learning difficulties and misconceptions found in the students concerning the theme of CE. Thus, several positive indicators were collected regarding the operation of the FACE approach in classroom context. These findings point to the practical relevance of the theoretical assumptions related to its construction, such as the plan for facilitating abstraction by the use of analogies and simultaneous simulation of events at the macro, submicro and symbolic levels.

So, this study has revealed several hints that FACE approach promotes facilitated abstraction in a classroom context. However, it should be recalled that we have not carried an experimental study, thus we cannot guarantee, or even conclude, that the improvement found in the results is due to the use of the FACE approach. The results could have been affected, for instance, by the fact that the students have solved the same questionnaire for a second time. Even though an alternative version was created in order to minimize this effect, repeating the test and re-learning the same subject by another means may have made a difference in terms of the improvements noticed. This is one of the reasons why we have already mentioned that this case study was designed to obtain preliminary information about the use of FACE approach in its context. The conclusions are presented as being indicative, without the intention of establishing direct cause and effect relationships or generalization. However, the information resulting from this study is expected to provide a guideline for the reformulation of the FACE approach and some ideas to explore/confirm in future studies. The triangulation of the sources of data collection, including the cross-referencing with the components of FACE approach, constituted a mean to ensure the internal validity of the results obtained.

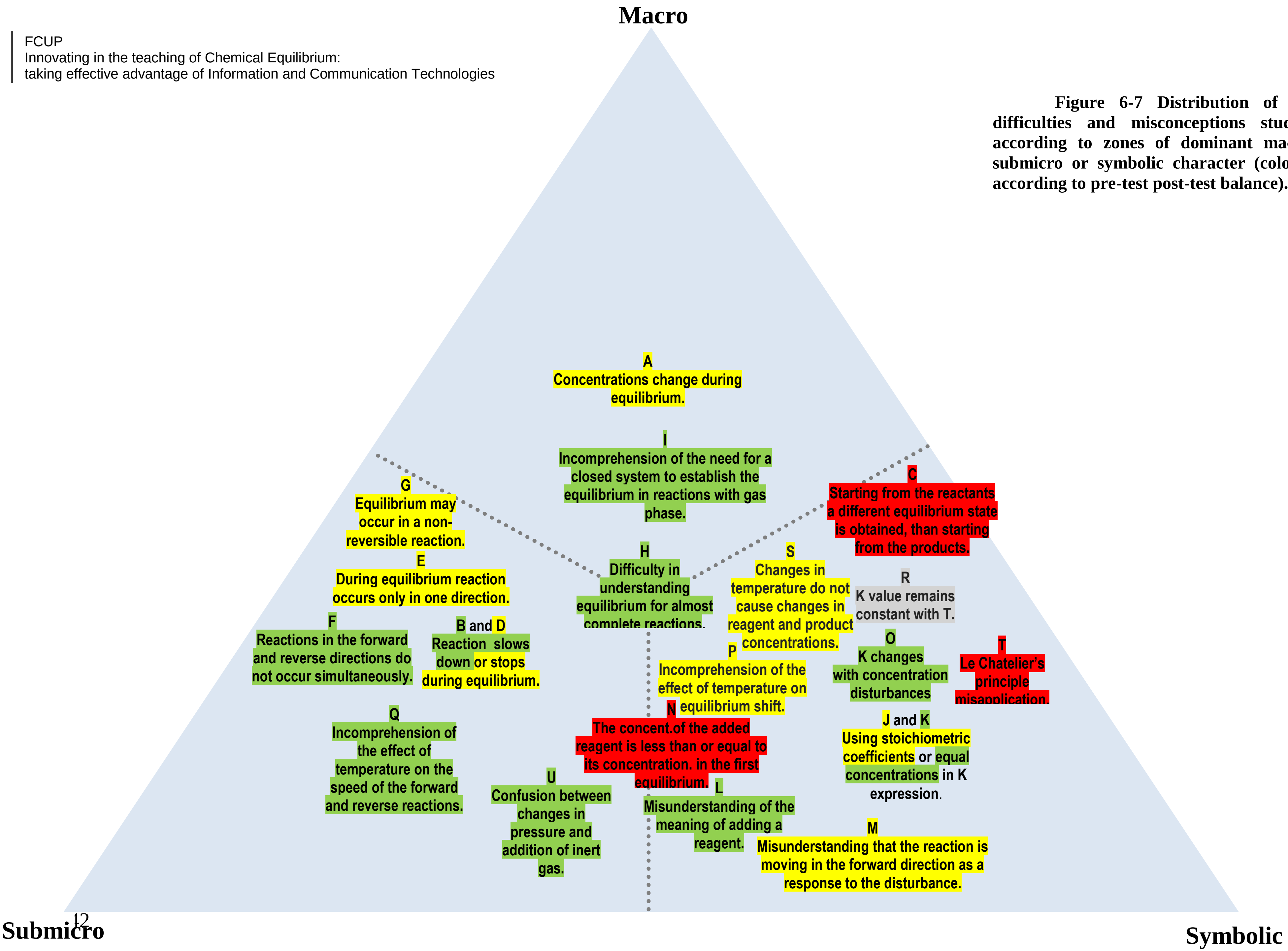
It is important to highlight the role of the teacher since the observation notes have signed that the interaction with the students throughout the activities, the monitoring of the process of knowledge construction and the promotion of reflection about the questions in the exploration guide are essential to the good outcome of the approach. Thus, it is important to consider the construction of a teacher's guide, which should include the difficulties that the approach is prepared to work on, referring in particular to the activity of the exploration guide and the elements of the simulation that facilitate the process of abstraction in each category.

From stage of analysis IV, we can verify that we have good results for categories related to the microscopic representation and the macro analogy with the reactor. Nevertheless, in what concerns to the symbolic level, elements of the simulation sometimes are related to good results and other times, even combined with the activities of the exploration guide, seem to be insufficient to overcome the barriers and destroy the misconceptions. Figure 6.7 recovers the triangle we have developed in Chapter 3, applying it to the difficulties that were treated in this study, using colors according to the results obtained for each category. As we have noticed in previous chapters the symbolic level is considered the most abstract. Thus, it is no surprise to find that the alternative conceptions concerning this domain appear to more resistant to change. They imply a high capability of abstraction, which FACE approach was not able to help students reach. In the next chapter, a list of recommendations for the reformulation of FACE approach will be presented according to these findings.

Another interesting aspect from the results, which is in accordance with the literature review, is that Le Chatelier's principle seems to be a double-edged sword. In the one hand students retain the idea of the system counteracting due to easily memorizing the principle. On the other hand, students fail to apply the principle correctly and end up using the language characteristic of one type of disturbance in other forms of disturbing equilibrium.

In favor of diminishing blank answers we had the fact that this investigation was useful for the respondents (Carmo & Ferreira, 1998) because it is one of the contents of their evaluation in the curriculum of Physics and Chemistry. However, this fact did not prevent some students from responding “the same answer for the other test” recognizing similar questions and showing lack of persistence in improving knowledge. Also, some blank answers in the exploration guide, in a sample which categorization reveals to be mainly constituted by interested students, exposes that it is important to reformulate this resource, especially in the extension and perhaps including tips for helping students in the conclusions and reflections.

Figure 6-7 Distribution of the difficulties and misconceptions studied according to zones of dominant macro, submicro or symbolic character (colored according to pre-test post-test balance).



Although the simulation appears to be appellative, students have to be encouraged to reflect and draw conclusions. Reserving more than 90 minutes for the activity and/or reducing the number of activities on the exploration guide constitute two possible suggestions. We have noticed some dispersion in the beginning of the exploration of the simulation, which was minimized when students started to follow the exploration guide.

In what concerns to the difficulties initially present in the sample, it is interesting to remark that both the most present and the more absent categories were related to temperature disturbances. Although the students had the idea that temperature affects equilibrium constant, they were not able to understand the effect of temperature in the shift of the equilibrium and in the velocity of the reactions. As exposed in the previous section, these difficulties were reduced after FACE approach application but still prevail in a generous group of students. The understanding of the effect of temperature in the disturbance of CE, implies combining data from different sources and relating information, involving a diversity of mental processes connected to abstraction (Chapter 5).

In order to answer the questions that were posed at the beginning of this investigation we have collected data on how the approach works in promoting facilitated abstraction in the classroom context. Several indicators demonstrated the relevance of the theoretical assumptions underlying the construction of FACE approach, namely the confirmation that students have common misconceptions, the importance of the analogies and microscopic representation as well as the different levels of information. Based on the results, especially the final stage (IV) we are able to define some conditions, in the case under study, that promote facilitated abstraction by the use of computational resources and trace some suggestions for the reformulation of face approach as well as a list of recommendations for the use of ICT in the teaching of CE. This will be the focus on Chapter 7.

Chapter 7 - Outcomes of the project

7.1. FACE approach and suggestions for reformulation

The approach for facilitating abstraction in the learning of Chemical Equilibrium presented in this dissertation is intended to constitute itself one of the outcomes. As discussed in Chapter 6 the results have pointed pedagogical relevance in the approach, revealing that several of its features can facilitate the attainment of the level of abstraction necessary to understand the concepts in Chemical Equilibrium and reduce difficulties/misconceptions commonly found during the teaching of this thematic.

The results indicated that the following elements constitute important conditions for facilitating abstraction in the learning of Chemical Equilibrium:

- representation of the submicro level using analogies;
- simultaneous coverage of the events at the three levels (micro, macro and symbolic);
- confrontation of the students' previous ideas with the results from the simulation, this being promoted by the exploration guide and the teacher.

Nevertheless, in face of the results obtained we admit that there are perspectives for improving the results and design a more prospective approach. Also, the technologic field is a domain in quick evolution so it is important to refresh the content of the approach on the light of new tendencies. In this perspective we have organized our intentions concerning FACE approach according to the categories and findings from Chapter 6 (Table 7.1).

Table 7-1 Suggestions for the reformulation of the FACE approach in face of the case study's results.

Category		Face response	Implications for teaching strategies concerning mental process involved in abstraction	Suggestions for reformulation
A	**The concentration of reagents and / or products changes during equilibrium state.**	Face response was positive. The simulation directly shows the concentrations of equilibrium remaining constant and the exploration guide questions the student about this fact having the large majority answered correctly. Nevertheless, an even better result was expected in this category from pre-test to post-test.	New concepts need to be anchored in the concepts of a pre-existing network in long term memory.	Ask students to directly register quantities of reactants and products in equilibrium as soon as it is attained and a few seconds later in order to favor the verification of equality, helping the idea to prevail in long term memory. A graphical element in the simulation could also help to verify the maintenance of concentrations although it would also increase the complexity of the simulation.
B	**The reaction rate decreases in equilibrium state.**	The permanence of the motion of the particles associated to the question that reflects upon this fact seems to provide very good results in avoiding the idea that the reaction rate decreases during equilibrium.	Appeal to analogies in order to establish metaphors with more concrete concepts. Use simulations to represent/interact with models, assisting mental abstraction and analogical inferences.	Maintain the analogy used in the microscopic representation.
C	**Starting from the reactants a different equilibrium state is obtained, than starting from the products.**	Although one of the activities from the exploration guide is dedicated to this idea and the simulation clearly allows verifying that the same quantities are obtained, the results from the tests are not positive. Some answers to the exploration guide suggest that although students recognize that the same quantities are achieved, the industrial production will be different starting from products or reactants (could this have been the confusing factor?). Should the exploration guide be smaller to avoid blank answers by the end? Is it worth it to dedicate an entire activity to this category?	Establish a sequence to approach the different levels from chemistry knowledge (due to the need to perform shift in attention and limited capacity of memory working space).	The activity from the exploration guide should be reformulated to improve the shift of attention to the essential components of the simulation in this category. Also, since only two students revealed this misconception, it is not one of the central topics from the curriculum, and students memory working space is of limited capability it should be considered the possibility of not dedicating an entire activity to this category.

Category		Face response	Implications for teaching strategies concerning mental process involved in abstraction	Suggestions for reformulation
D	**Reaction stops during equilibrium.**	The continuation of the motion of the particles associated to the question that reflects upon this fact provides good results in the exploration guide although some resistance to this idea prevails in the post-test.	Minimize the absence of concrete experiences using representations that support the ideas.	The zoom of the microscopic representation should clearly evidence the simultaneous formation of products and reactants instead of only showing the movement of particles. Using this new feature it would be interesting to include a question in the exploration guide for categories E and F.
E	**Reaction occurs during equilibrium, but only in one of the directions.**	Results but could be better, perhaps due to the lack of a short answer question concerning this idea in the exploration guide.	Minimize the absence of concrete experiences using representations that support the ideas. Encourage students to reflect on events and predict responses in order to expose relationships.	Upgrade to a blinking arrow in both directions during equilibrium to give the idea of reactions permanence and simultaneity. Improve the zoom representation. Include a short answer question concerning this idea in the exploration guide.
F	**Reactions in the forward and reverse directions do not occur simultaneously.**	The simulation of the microscopic constant movement, with “dot color mixing”, appears to eliminate the idea of compartmentalized view of chemical equilibrium.	Appeal to analogies in order to establish metaphors with more concrete concepts. Use simulations to represent/interact with models, assisting mental abstraction and analogical inferences.	Maintain the analogy used for simulating microscopically the evolution to equilibrium.
G	**Equilibrium may occur in a non-reversible reaction.**	Actions in the simulation, especially disturbances allow students to consolidate the idea of reversibility as being connected to equilibrium reactions. Nevertheless, some students still fail in this category in the post-test.	Provide different explanations for the same concept.	Adding new reactions to the simulation that cover these aspects would enrich FACE approach. Nevertheless, cost/benefit should be pondered since this is a meticulous process of construction and the results are already satisfactory. Also, increasing the complexity of the simulation could turn itself against us, since facilitating abstraction is the purpose. Focusing this category in the reflection made by the teacher at the end of the activity is also an alternative.

Category		Face response	Implications for teaching strategies concerning mental process involved in abstraction	Suggestions for reformulation
H	**Difficulty in understanding equilibrium for almost complete reactions.**	The diversity of values and different equilibrium constants students observe and register along the approach appear to enlarge their view about the multiplicity of equilibrium states possible.	Follow the multiple representation principle. Minimize the absence of concrete experiences using representations that support the ideas.	The results point for the importance of the quantitative elements of the simulation.
I	**Incomprehension of the need for a closed system to establish the equilibrium in reactions with gas phase.**	Actions in the simulation allow students to get familiar with a gaseous system in a closed reactor, where equilibrium is established.	Relate different levels of description of a concept (macro, micro, symbolical). Importance of applying concepts in context, so that knowledge acquires real meaning.	Results point the importance of the macroscopic analogy with a reactor.
J	**Confusion between equilibrium concentrations and stoichiometric coefficients.**	Face approach has partially improved results in a category where several students revealed difficulties. Nevertheless, although students register correct values in the exploration guide, this activity does not seem to create sufficient conflict to promote conceptual change in most of the students that reveal the difficulty, reason why several students still fail in post-test question about this category.	New concepts need to be anchored on the concepts of a pre-existing network in long term memory. Help to mobilize previous abstractions and consider them as the base for new abstractions during the design of teaching strategies.	Ask students to obtain the value of *K* from the concentrations forcing them to reflect on how to calculate equilibrium constant, instead of only registering the values in order to promote conceptual change. The quantity of students that reveal this difficulty justifies the investment of time for this category in the exploration guide.
K	**At equilibrium the total concentrations of products and reagents are the same.**	Face approach has considerably improved results.		Results are good pointing once again the importance of the quantitative elements of the simulation. Nevertheless, suggestion made for category J could also help in this category.

Category		Face response	Implications for teaching strategies concerning mental process involved in abstraction	Suggestions for reformulation
L	**Misunderstanding of the meaning of adding a reagent.**	Students recognize that system displacement is in the forward direction when adding a reactant, which justifies the good results in the post-test. Nevertheless, in the exploration guide several students include the information that the system shifts in the direction of the smaller number of gaseous moles, confusing this disturbance with changes in pressure. Pressure changes are worked upon in a previous activity in the exploration guide, which has certainly contributed to the confusion. Also students reveal to be very familiar with the language referring to changes in pressure.	Promote student's active learning. Teacher must guide the student in the process from concrete to abstraction.	Clearly specify the kind of disturbances treated in each activity of the exploration guide. Be aware of Le Chatelier's principle misapplication.
M	**Misunderstanding that the reaction is moving in the forward direction as a response to the disturbance.**	Most students answer correctly to the exploration guide but, again, exploring the simulation and answering as expected to the exploration guide seems to be insufficient to destroy misconceptions in several students.	New concepts need to be anchored on the concepts of a pre-existing network in long term memory. Teacher must guide the student in the process from concrete to abstraction. Help to mobilize previous abstractions and consider them as the base for new abstractions during the design of teaching strategies.	The teacher should reinforce the reflection promoted by the exploration guide, assuring that students interiorize the verifications and conclusions proposed in the exploration guide.
N	**The equilibrium moves in the forward direction, so in the new equilibrium state the concent. of the added reagent is less than or equal to its concentration. in the first equilibrium.**	Typical situation where students answer correctly to the exploration guide and register the conclusion proving that they notice that the quantity of reagent is superior in second equilibrium. Nevertheless, they fail to answer correctly in the post –test. This specific case appears to be related to the use of Le Chatelier's principle typical language.	Clarify simplifications / idealizations associated to a scientific model. Teacher must guide the student in the process from concrete to abstraction.	Clearly exposing that the response of the system according to Le Chatelier's principle does not signify consuming more reagent than the quantity added.

Category		Face response	Implications for teaching strategies concerning mental process involved in abstraction	Suggestions for reformulation
O	**The value of the equilibrium constant can be altered by addition of reagent.**	Face approach provide good results in a category present in several students.	Promote student’s active learning. New concepts need to be anchored on the concepts of a pre-existing network in long term memory.	The quantitative analysis of equilibrium displacements using *Q* and *K* values (available in the simulation) combined with the registration in the exploration guide appears to be sufficient to promote conceptual change in this category.
P	**Incomprehension of the effect of temperature in the direction of equilibrium displacement.**	Face approach has partially improved results in categories where a large number of students revealed difficulties. The fact that several elements of the simulation have to be crossed in this category can justify the difficulties. Students must consider kinetics, equilibrium law, enthalpy, system composition and Le Chatelier´s principle in order to deal with all the aspects from temperature disturbances. This can clearly overload memory working space and implies abstracting over previous abstractions.	Should be given numerous opportunities to relate the three representations so that multiple linkages are formed in long-term memory. Establish a sequence to approach the different levels of chemical knowledge. Help to mobilize previous abstractions and consider them as the base for new abstractions during the design of teaching strategies.	Reformulate the activity related with temperature disturbances in the exploration guide in order to establish a sequence to deal with all the aspects from temperature disturbances (constructing the knowledge step by step could facilitate abstraction).
Q	**Incomprehension of the effect of temperature on the speed of the forward and reverse reactions.**			
R	**The value of the equilibrium constant cannot be changed by the temperature variation.**	Students from the sample had already acquired the idea that *K* changes with the temperature.	------	------
S	**Changes in temperature do not cause changes in reagent and product concentrations.**	Face approach has partially improved results.	Promote student’s active learning. New concepts need to be anchored on the concepts of a pre-existing network in long term memory	Include this category in the steps predicted in the reformulation of categories P and Q.

Category		Face response	Implications for teaching strategies concerning mental process involved in abstraction	Suggestions for reformulation
T	**The decrease in volume is counteracted by the displacement of the equilibrium towards the formation of the largest number of gaseous moles.**	Students continue to apply Le Chatelier's principle to volume variations even after FACE approach, one of the categories with the worst response.	Promote student's active learning. New concepts need to be anchored on the concepts of a pre-existing network in long term memory. Clarify simplifications / idealizations associated to a scientific model.	Clearly exposing that the response of the system according to Le Chatelier's principle does not signify consuming more reagent than the quantity added. Ponder the inclusion of Le Chatelier's principle limitation in the exploration guide.
U	**The addition of inert gas increases the pressure whereby the system moves towards the formation of the least number of gaseous moles (misunderstanding that the addition of inert gas does not affect equilibrium in ideal systems).**	For this category it seems that the activity from the exploration guide caused some misunderstanding in the students, since they were able to improve in the post-test but registered wrong data in the exploration guide.	Help to mobilize previous abstractions and consider them as the base for new abstractions during the design of teaching strategies. Present the convenience/evidence for extending a concept to new domains.	Reformulate this activity in the exploration guide, considering the possibility of combining this actions with the activity related with pressure change in order reduce the extension of the exploration guide and avoid blank answers registered close to the end.

With regard to the dissemination of this outcome, FACE pedagogical approach, the first idea was to integrate it into a reference portal dedicated exclusively to Chemical Equilibrium. Since this work was developed over several years, naturally we have reflected along the process. In recent years file-sharing platforms such as generalist Moodle’s and blogs of Physics and Chemistry, have become more attractive for the teachers. Although we intend to ultimately reach the students, teachers constitute our first target since they are the ones who can guide the students through the process of facilitating abstraction. This guidance is, as results and references have pointed, essential for the success of the strategy. So, we plan to upload FACE approach in several generalist national and international platforms for the teaching of chemistry and sciences, where users can also share their files and communicate, following the new tendencies described in Chapter 4. This intention is not impeditive of maintaining the simulation available online in a “private” location with a renewed visual. The upload in science teaching platforms will guarantee the Web 2.0 component, important for improving the resources and reach a larger community.

To close this section, we present the elements to be included in the reformulated version of the simulation, which appear in blue colour in a Figure 7.1. This figure represents an upgrade of the triangle presented in Chapter 5 and allows easy verifying of the improvement in the coverage of all three levels of knowledge predicted for the new version of the simulation. Table 7.2 summarizes aspects to reformulate in FACE approach.

Table 7-2 Summary of the aspects to reformulate in FACE approach

Notes for the reformulation of the Simulation

- Maintain the submicro representation based on molecular movement and improve the zoom element in order to effectively represent the simultaneous formation of reagents and products during equilibrium state.
- Ponder the inclusion of a simple graphical element in the simulation to present the change in quantities over time.
- Importance of the coverage of the three levels (macro, submicro and symbolic), helping students to construct an unified vision of the phenomenon.

Notes for the reformulation of the Exploration Guide

- Activity 1 – Ask students to directly register the quantities at equilibrium state after some time is passed from the establishment; include a question concerning the fact that the reaction occurs in both directions during equilibrium.
- Activity 2 - Reformulate this activity in order to establish a sequence to deal with all the aspects from temperature disturbances (constructing the knowledge step by step could facilitate abstraction).
- Activity 4 – Consider removing this activity and include some actions related to it in activity 1;
- Activity 5 - Simplify the actions from this activity in the exploration guide, considering the possibility of replacing it by confronting students with this disturbance (inert gas) in the reflections from activity 3, in order reduce the extension of the exploration guide and avoid blank answers registered close to the end.
- Include an activity where students are asked to perform calculations, such as equilibrium constant, since several students reveal this difficulty;
- Clearly identify the disturbance behind each activity.
- Ponder the inclusion of Le Chatelier’s principle limitation in the exploration guide.
- Reduce the extension of the exploration guide by limiting the number of difficulties to work on based on curricular relevance.

General notes

- The teacher should reinforce the reflection promoted by the exploration guide, assuring that the students interiorize the verifications and conclusions proposed, especially for the categories that have revealed more resistance in the study. Auxiliary materials should include this information.
- The teacher should beware of common misapplication of Le Chatelier’s principle delimitating the frontiers and conditions for its appliance.

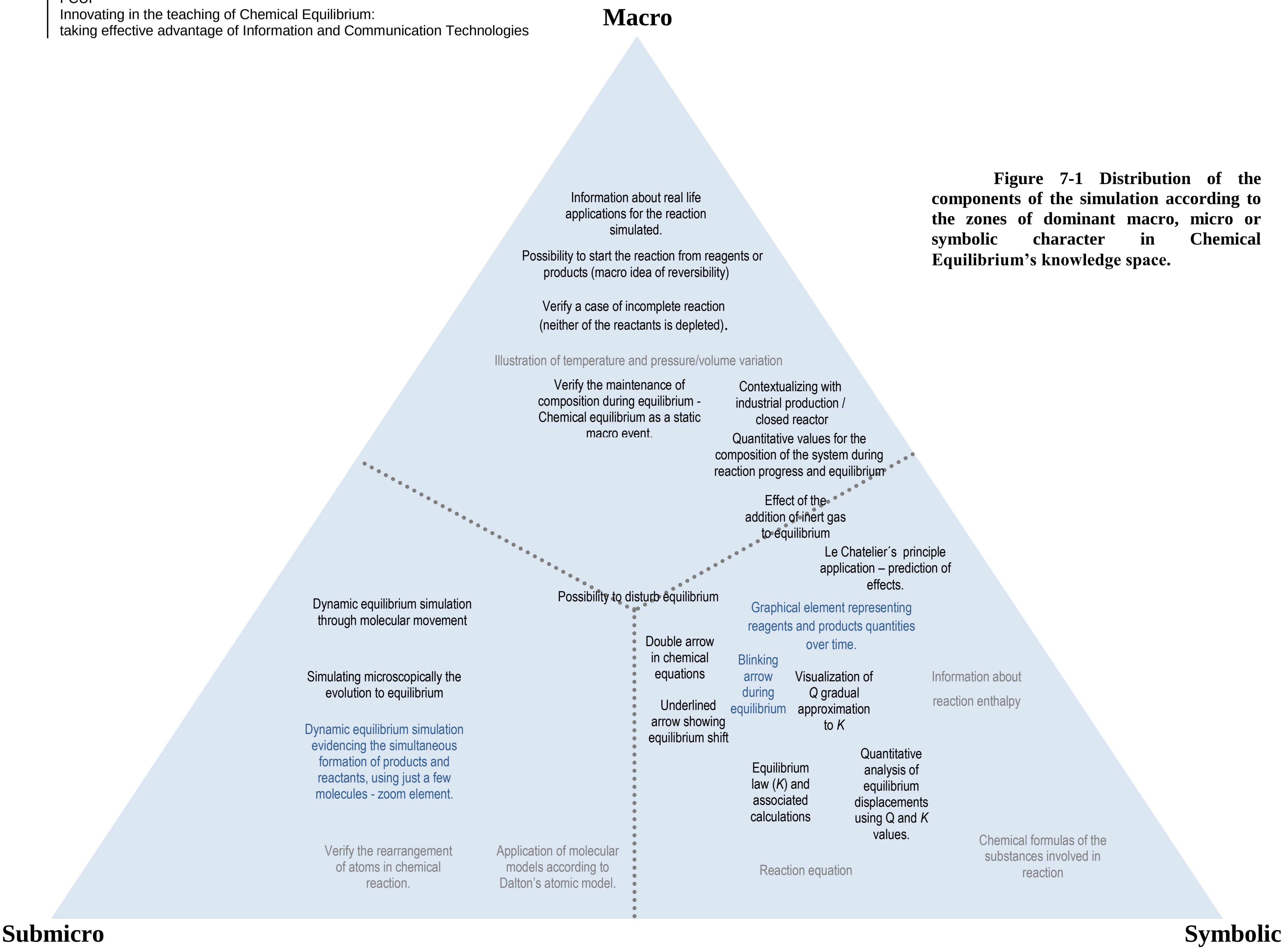


Figure 7-1 Distribution of the components of the simulation according to the zones of dominant macro, micro or symbolic character in Chemical Equilibrium's knowledge space.

7.2. Recommendations for the use of digital resources in the teaching of Chemical Equilibrium

As we have referred, this project was developed in collaboration with CROSSNET. Three sub-cases constituted contributions for the national case study concerning the project, whose structure was previously defined. These cases were associated to the overcoming of barriers in order to reach active learning, learning in context and facilitated abstraction. The cases that studied active learning and learning in context were conducted by fellow chemistry teachers: António Ferreira and João Vale, who cooperated with us in CROSSNET project. All the approaches were based in the use of digital resources.

Having performed a transversal analysis of the three cases in order to present the results of the project (Paiva & Fonseca, 2012) several indicators have shown up that students were motivated and learned effectively, safeguarding that the conditions under which ICT are applied constitute an essential influence in the process. It is also important to refer that the computational approaches should be considered as a positive contribution but not a “miracle solution” to solve all the teaching/learning problems.

From the results obtained, under the conditions, that these studies were conducted, we conclude that it is valuable to construct approaches for the teaching of Chemical Equilibrium based on the use of ICT. They also point the importance of identifying the barriers to work on and considering the appropriated teaching and learning theories/ methodologies as well as the results from previous investigations.

Reflections on the work done, also remark the relevance of defining the essential topics to be learnt and the need to limit the number of difficulties/misconceptions to minimize. This is because we can “lose sight” of our purpose in such a way that retaining the essential becomes difficult.

The importance of the representative capabilities and the possibilities of interaction provided by some computational resources to the teaching of complex concepts is reinforced by this study. The digital resources also motivate students minimizing some possible resistance due to the formality of the concepts.

In the ideas just mentioned, we have found implicit several conditions under which computational resources can be useful for the teaching/learning of Chemical Equilibrium. This was one of our aims for the project, directly related to the central question of the national case study. Next table resumes the conditions, constituting one of the outcomes of our work in CROSSNET (Paiva & Fonseca, 2012).

Table 7-3 Important conditions about the use of ICT in the teaching of Chemical Equilibrium (adapted from Paiva & Fonseca, 2012).

Recommendations for using ICT approaches in teaching Chemical Equilibrium	Indicators in the study
Identify the barriers to work on according to **priorities** and beware of the obstacles.	Defining a priority and designing the strategies for the transposition of an obstacle led to good results.
Take advantage of multimedia capabilities provided by ICT for **applying STS perspective** in the classroom.	STS perspective (in accordance to the interdisciplinary nature of Chemical Equilibrium) linked to goal achievement motivated the students.
Plan the lesson to allow students cooperation in the exploration of the resources.	Inter-student cooperation was positive, they had to exchange ideas and negotiate the exploration of the resources/ design of the products.
Encourage students to confront common **misconceptions and learning difficulties** with model simulations, guiding them with a support material like an exploration guide.	Having encouraged students to face common misconceptions through the exploration guide contributed to a minimization of errors.
Define the essential topics to be learnt and select the difficulties to work on; focus on minimizing a small number of misconceptions.	The exploration guide and post-test seemed to demand too much information. We can “lose sight” not retaining the essential.
Keep in mind: • **the representative capabilities (microscopic model),** • **opportunities for interaction,** • **motivational elements,** • **graphics and organization** when constructing / selecting a **resource.**	Reformulation suggestions for the resources include reinforcements in representation of events and interaction. Representative capabilities are directly related to the process of facilitating abstraction. Motivation is important to avoid resistance due to formal concepts.
Design **quality support materials** for guiding the students. Attention must be paid to the **promotion of self-regulation and fighting initial dispersion**.	Exploration guides balance the “liberty” allowed by the use of ICT. Could the use of a check-list be useful for self-regulation?
Provide a meaningful experience for the students: show the **purpose of the activity**; **be permanently supportive** during the exploration **and stress main ideas** at the end.	Observations indicated that explaining activities, interacting with the students and summarizing ideas can avoid unnecessary misunderstandings.
Adapt the support materials for the students, the school and the time available.	Time constraints and technical difficulties appeared in all cases.

Our work in CROSSNET project, also envisaged the enlargement of teachers' vision so that they can be aware of some of the barriers present in education, particularly in Chemical Equilibrium, and the development of skills in order to cross these boundaries by using computational resources. From the experiences of the teachers collaborating in the study several recommendations can be traced (Table 7.4).

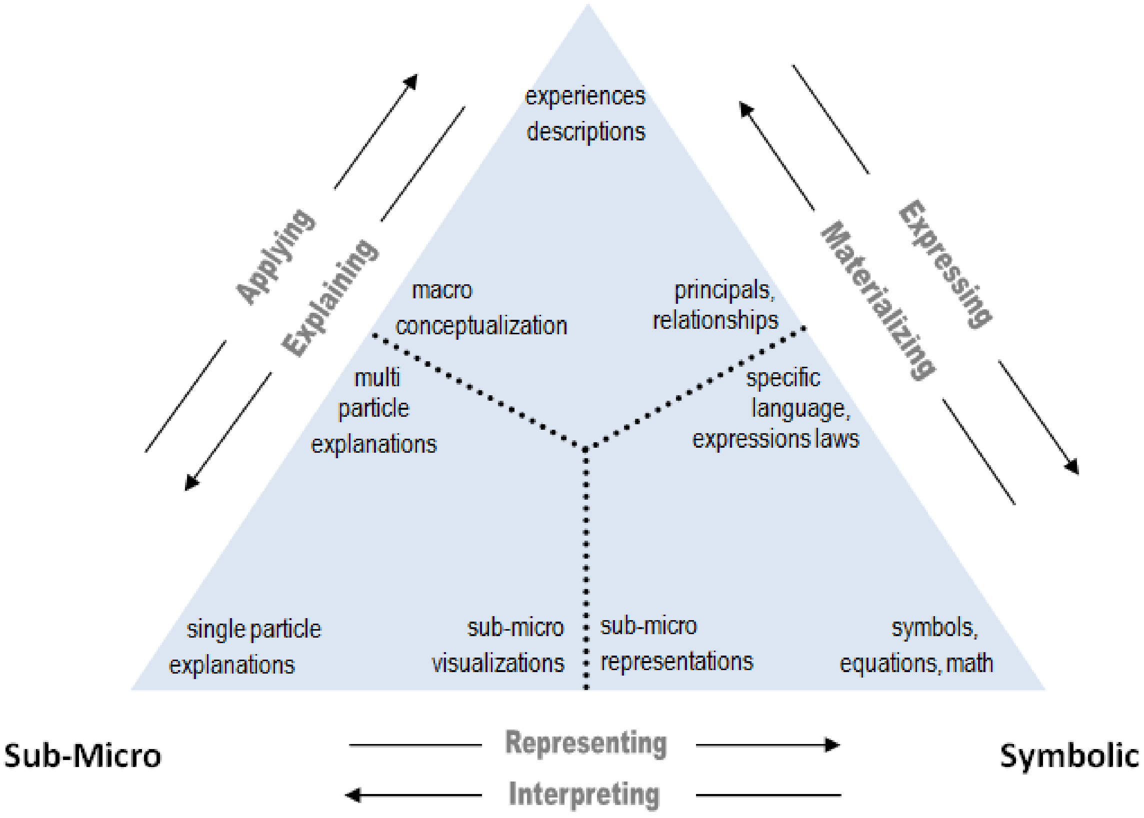
Table 7-4 Recommendations about Teacher Education / Pedagogical Practice (adapted from Paiva & Fonseca, 2012).

Recommendations based on the use of ICT for teaching Chemical Equilibrium		
Teacher's Role		
Preparation	**Intervention**	**Reflection**
• Define the essential topics to be explored through the use of ICT, separating the essential from the accessory; • Be aware of learning difficulties and misconceptions in the field. • Identifying the barriers to transpose and considering the results from educational researches; • Plan to promote facilitated abstraction, active and in-context learning of Chemical Equilibrium. • Plan according to time constraints; • Careful in-school preparation to prevent technical problems: internet access, computer functionality and availability. • Select, adapt and construct appropriate support materials to guide students along the exploration of central resources. • If links are involved, verifying the maintenance of the contents online. • Prefer resources that integrate pedagogical and scientific qualities, as well as communication ones: - Representation of events (simulation). Interaction - Motivational elements; - Relevant Information	Introduce the type of resources in use, especially when it is not usual to apply them in the class. Permanent interaction with students to avoid dispersion form the goals and misinterpretations. Value positive interactions between students and avoid passive roles within working groups. Elucidate the evaluation parameters for the activity. Deal with time constraints.	Final discussion with students to summarize relevant conclusions and diagnose possible persistent misconceptions. Improvement of the approaches for further use.

7.3. Creative theoretical work presented in chapters 2 and 5.

7.3.1. Zones of chemistry knowledge space – an expansion to the scheme proposed by Johnstone (1991)

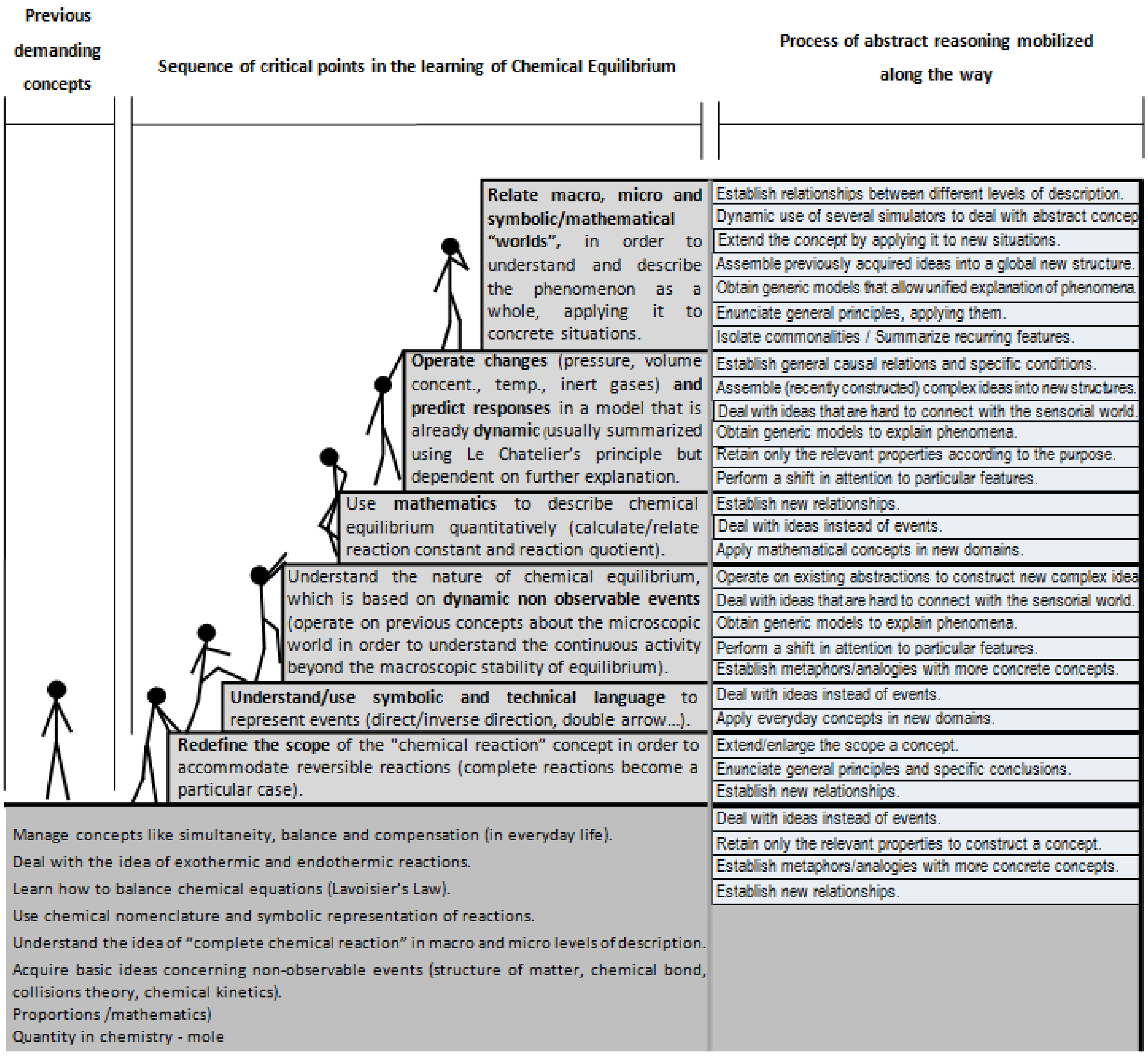
From the review presented in chapter 2, as well as the growing interest and experience of the group in the field, we have created an original diagram about the character of knowledge in chemistry. The original development of the triangle from Figure 2.9 – Zones of chemistry knowledge space – an expansion to the scheme proposed by Johnstone (1991) is intended itself to constitute one of the outcomes from this project.



As we have seen throughout the dissertation, this diagram can be useful to perform different analysis, namely the area of distribution of students' difficulties in a subject, the dependence of a scientific model from each of the three levels and the domain of incidence of a resource or teaching strategy.

7.3.2. Climbing the stairway of Chemical Equilibrium learning

In Chapter 5 we have made an incursion through the “meanings” of abstraction in several references. Later, based on our personal experience and considering the usual sequence and content involved in the teaching of CE (according to chemistry curricukum for high school chemistry), we have related the mental processes involved in abstraction to the steps necessary for the understanding of the model used in Chemical Equilibrium teaching. The result is a stairway that students have to climb in order to understand Chemical Equilibrium (Figure 5.1), which can be a useful tool for teachers.



Relate macro, micro and symbolic/mathematical “worlds”, in order to understand and describe the phenomenon as a whole, applying it to concrete situations.

Establish relationships between different levels of description.
Dynamic use of several simulators to deal with abstract concep
Extend the concept by applying it to new situations.
Assemble previously acquired ideas into a global new structure.
Obtain generic models that allow unified explanation of phenomena.
Enunciate general principles, applying them.
Isolate commonalities / Summarize recurring features.

Operate changes (pressure, volume concent., temp., inert gases) **and predict responses** in a model that is already **dynamic** (usually summarized using Le Chatelier's principle but dependent on further explanation.

Establish general causal relations and specific conditions.
Assemble (recently constructed) complex ideas into new structures.
Deal with ideas that are hard to connect with the sensorial world.
Obtain generic models to explain phenomena.
Retain only the relevant properties according to the purpose.
Perform a shift in attention to particular features.

Use **mathematics** to describe chemical equilibrium quantitatively (calculate/relate reaction constant and reaction quotient).

Establish new relationships.
Deal with ideas instead of events.
Apply mathematical concepts in new domains.

Understand the nature of chemical equilibrium, which is based on **dynamic non observable events** (operate on previous concepts about the microscopic world in order to understand the continuous activity beyond the macroscopic stability of equilibrium).

Operate on existing abstractions to construct new complex idea
Deal with ideas that are hard to connect with the sensorial world.
Obtain generic models to explain phenomena.
Perform a shift in attention to particular features.
Establish metaphors/analogies with more concrete concepts.

Understand/use symbolic and technical language to represent events (direct/inverse direction, double arrow…).

Deal with ideas instead of events.
Apply everyday concepts in new domains.

Redefine the scope of the "chemical reaction" concept in order to accommodate reversible reactions (complete reactions become a particular case).

Extend/enlarge the scope a concept.
Enunciate general principles and specific conclusions.
Establish new relationships.

Manage concepts like simultaneity, balance and compensation (in everyday life).
Deal with the idea of exothermic and endothermic reactions.
Learn how to balance chemical equations (Lavoisier's Law).
Use chemical nomenclature and symbolic representation of reactions.
Understand the idea of “complete chemical reaction” in macro and micro levels of description.
Acquire basic ideas concerning non-observable events (structure of matter, chemical bond, collisions theory, chemical kinetics).
Proportions /mathematics)
Quantity in chemistry - mole

Deal with ideas instead of events.
Retain only the relevant properties to construct a concept.
Establish metaphors/analogies with more concrete concepts.
Establish new relationships.

References

Abstraction. (n.d.). Retrieved May 22, 2017, from Oxford dictionary online: https://en.oxforddictionaries.com/definition/abstraction

Abstraction. (n.d.). Retrieved May 22, 2017, from Polish encyclopedia of Philosophy: http://peenef2.republika.pl/

Abstraction. (n.d.). Retrieved May 22, 2017, from Universal encyclopedia of Philosophy: https://pt.scribd.com/document/79752654/Abstraction-Universal-Encyclopedia-of-Philosophy

Abstraction. (n.d.). Retrieved May 22, 2017, from Encyclopedia Britannica online: https://www.britannica.com/topic/abstraction

Allsop, R. T., & George, N. H. (1984). Le Chatelier - a Redundant Principle? *Education in Chemistry, 21*, 54-56.

Alvarez, S. (2011). Chemistry: A Panoply of Arrows. *Angewandte Chemie , 51*, 590-600.

Angelelli, I. (2004). Adventures of Abstraction. *Poznaf Studies in the Philosophy of the Sciences and the Humanities, 82*, 11-35.

Araújo, C., Pinto, E., Lopes, J., Nogueira, L., & Pinto, R. (2006). *Estudo de caso.* Trabalho de Mestrado em Educação e Tecnologia Educativa, Universidade de Minho, Braga.

Atkins, P. W. (1998). *Physical Chemistry* (6th ed.). Oxford: Oxford University Press.

Aviram, A. (2000). From “Computers in the Classroom” to Mindful Radical Adaptation by Education Systems to the Emerging Cyber Culture. *Journal of Educational Change, 1,* 331-352.

Aviram, A. (2009). *No Proven Effectiveness, No Sustainable Change. Proposal for strategic approach to the computerization of education on the basis of 30 years of experience.* Retrieved May 5, 2010, from http://crell.jrc.ec.europa.eu/ICTeducation/Aviram.ppt

Azizoğlu, N., Alkan, M., & Geban, Ö. (2006). Undergraduate Pre–Service Teachers’ Understandings and Misconceptions of Phase Equilibrium. *Journal of Chemical Education, 83*, 825-834.

Bäck, A. (2014). *Aristotle's Theory of Abstraction.* Switzerland: Springer International Publishing.

Banerjee, A. C. (1991a). Misconceptions of Students and Teachers in Chemical Equilibrium. *International Journal of Science Education, 13*, 487-494.

Banerjee, A. C. (1991b). The Developement of Modules for the Teaching of Chemical Equilibrium. *International Journal of Science Education, 13*, 355-362.

Banerjee, A. C. (1995). Teaching Chemical Equilibrium and Thermodynamics in Undergraduate General Chemistry Courses. *Journal of Chemical Education, 72*, 879-881.

Barke, H., & Wirbs, H. (2002). Structural Units and Chemical Formulae. *Chemistry Education Research and Practice, 3*, 185-200.

Bergquist, W., & Heikkinen, H. (1990). Students Ideas Regarding Chemical Equilibrium. *Journal of Chemical Education, 67*, 100-103.

Bodner, G. M. (1991). I Have Found You an Argument: The Conceptual Knowledge of Beginning Chemistry Graduate Students. *Journal of Chemical Education, 68*, 385-388.

Bradshaw, D. E. (1988). Berkeley and Hume on Abstraction and Generalization. *History of Philosophy Quarterly, 5*, 11-22.

Bragin, V. (1996). Interactive Computer Visualization in the Introductory Chemistry Curriculum. *Journal of Chemical Education, 73*, 747-748.

Brown, T., Bursten, B., LeMay, H., Murphy, C., & Woodward, P. (2012). *Chemistry: The Central Science* (12th ed.). U.S.A.: Prentice Hall.

Carmo, H., & Ferreira, M. M. (1998). *Metodologia da Investigação.* Lisboa: Universidade Aberta.

Cartwright, N. (1983). *How the Laws of Physics Lie.* Oxford: Clarendon Press.

Cassel, C., & Symon, G. (2004). *Essential Guide to Qualitative Methods in Organizational Research.* London: SAGE Publications.

Chalmers, A. F. (2000). *Qué es esa cosa llamada ciência?* (3rd ed.). Madrid: España Editores.

Chang, R. (2005). *Química* (8th ed.). Madrid: McGraw Hill.

Cheung, D. (2009). The Adverse Effects of Le Châtelier's Principle on Teacher Understanding of Chemical Equilibrium. *Journal of Chemical Education, 86*, 514-518.

Christensen, L. (2007). *The Hands-On Guide to Science Communication.* New York: Springer-Verlag.

Christensson, C., & Sjöström, J. (2014). Chemistry in Context: Analysis of Thematic Chemistry Videos Available Online. *Chemistry Education Research and Practice, 15*, 59-69.

Christoff, K., & Keramatian, K. (2007). Abstraction of Mental Representations: Theoretical Considerations and Neuroscientific Evidence. In S. Bunge, & J. D. Wallis (Eds.), *Perspectives on Rule-Guided Behavior* (pp. 107-126). New York: Oxford University Press.

Çimer, A. (2007). Effective Teaching in Science: A Review of Literature. *Journal of Turkish Science Education, 4,* 20-44.

Crespo, R. F. (2009). "Nancy Cartwright, Millian and/or Aristotelian". *Sapientia, 65,* 225-226.

Crosland, M. P. (1959). The Use of Diagrams as Chemical 'Equations' in the Lecture Notes of William Cullen and Joseph Black. *Annals of Science, 15,* 75-90.

David, C. W. (1988). An Elementary Discussion of Chemical Equilibrium. *Journal of Chemical Education, 65,* 407-409.

de Jong, O., & Taber, K. S. (2014). The Many Faces of High School Chemistry. In N. Lederman, & S. K. Abell (Eds.), *Handbook of Research in Science Education* (pp. 457-480). New York: Routledge.

Descombe, M. (1998). *The Good Research Guide.* Buckingham: Open University Press.

Devetak, I., Vogrinc, J., & Glažar, S. (2009). Assessing 16-Year-Old Students' Understanding of Aqueous Solution at Submicroscopic Level. *Research in Science Education, 39,* 157-179.

Dodge, B. (1997). *Some Thoughts About WebQuests.* Retrieved June 12, 2004, from http://edweb.sdsu.edu/courses/edtec596/about_webquests.html.

Dubinsky, E. (2002). Reflective Abstraction in Advanced Mathematical Thinking. In D. Tall (Eds.), *Advanced Mathematical Thinking* (pp. 95-126). New York: Kluwer Academic Publishers.

Dumon, A., & Mzoughi-Khadhraoui, I. (2014). Teaching Chemical Change Modeling to Tunisian Students: an "Expanded Chemistry Triplet" for Analyzing Teachers' Discourse. *Chemistry Education Research and Practice, 15,* 70-80.

Erdemír, A. Ö., Geban, Ö., & Uzuntiryaki, E. (2000). Freshman Students' Misconceptions in Chemical Equilibrium. *Journal of Chemical Education, 18,* 79-84.

Fiolhais, C., Festas, I., & Damião, H. (2014). *Programa de Física e Química A – 10.º e 11.º anos. Curso Científico-Humanístico de Ciências e Tecnologias.* Lisboa: Ministério da Educação e Ciência.

Fonseca, S. (2006). *Influência de Gases Inertes no Equilíbrio Químico: Nuances e Simulações Computacionais. Tese de Mestrado em Educação Multimédia.* Porto: Universidade de Porto.

Fonseca, S., & Paiva, J. (2006). EquilibrAction - Using Computational Resources Potential to Cross Boundaries in the Teaching of Chemical Equilibrium. *CROSSNET Meeting.* Kiel.

Fonseca, S., & Paiva, J. (2007). EquilibrAction – Participação Portuguesa no Projecto Europeu CROSSNET. *5º Encontro DEDQ.* Braga.

Fonseca, S., & Paiva, J. (2010). Inovar no Ensino do Equilíbrio Químico por Recurso a Abordagens TIC Facilitadoras da Abstração. *1º Encontro Internacional TIC e Educação - TIC Educa.* Lisboa.

Fonseca, S., Paiva, J., & Gonçalves, J. (2005). Protótipo de uma Simulação Computacional sobre Equilíbrio Químico para o Ensino. *4º encontro DEDQ.* Lisboa.

Fonseca, S., Paiva, J., Ferreira, A., & Vale, J. (2008). Portuguese Participation in CROSSNET: “EquilibrAction” National Project. *XXI SPQ Meeting.* Porto.

Furió, C., Calatayud, M. L., Bárcenas, S. L., & Padilla, O. M. (2000). Functional Fixedness and Functional Reduction as Common Sense Reasonings in Chemical Equilibrium and in Geometry and Polarity of Molecules. *Science Education, 84*, 545-565.

Gabel, D. (1993). Use of the Particle Nature of Matter in Developing Conceptual Understanding. *Journal of Chemical Education, 70*, 193-194.

Gabel, D. (1999). Improving Teaching and Learning through Chemistry Education Research: A Look to the Future. *Journal of Chemical Education, 76*, 548-554.

Ganaras, K., Dumon, A., & Larcher, C. (2008). Conceptual integration of Chemical Equilibrium by Prospective Physical Sciences Teachers. *Chemistry Education Research and Practice, 3*, 240-249.

Gilbert, J. K. (2005). Visualization: A Metacognitive Skill in Science and Science Education. In J. K. Gilbert (Eds.), *Visualization in Science Education* (pp. 9–27). The Netherlands: Springer.

Gilbert, J. K., & Treagust, D. (2009). *Multiple Representations in Chemical Education.* The Netherlands: Springer.

Gil-Pérez, D., Guisasola, J., Moreno, A., Cachapuz, A., Carvalho, A., Torregrosa, J., et al. (2002). Defending Constructivism in Science Education. *Science & Education, 11*, 557–571.

Godfrey-Smith, P. (2009). Abstractions, Idealizations, and Evolutionary Biology. In A. Barberousse, M. Morange, & T. Pradeu (Eds.), *Mapping the Future of Biology: Evolving Concepts and Theories* (pp. 47-56). The Netherlands: Springer.

Grapí, P. (2011). The Role of Chemistry Textbooks and Teaching Institutions in France at the Beginning of the Nineteenth Century in the Controversy About Berthollet's Chemical Affinities. In R. Witje, & P. Heering (Eds.), *Learning by Doing: Experiments and Instruments in the History of Teaching* (pp. 55-70). Stuttgart: Franz Steiner Verlag.

Griffiths, A. K. (1994). A Critical Analysis and Synthesis of Research on Students' Chemistry Misconceptions. In H. Schmidt (Ed.), *Proceedings of the 1994 International Symposium Problem Solving and Misconceptions in Chemistry and Physics* (pp. 70-99). The International Council of Association for Science Education Publications.

Hackling, M. W., & Garnett, P. J. (1985). Misconceptions of Chemical Equilibrium. *European Journal of Science Education, 7*, 205-214.

Hadenfeldt, J., & Neumann, K. (2014). Understanding Matter - A Review of Research on Students' Conceptions of Matter . *NARST 2014.* Pittsburgh.

Halim, N. A., Ali, M., Yahaya, N., & Haruzuan, M. (2013). Mental Model in Learning Chemical Bonding: A Preliminary Study. *Procedia - Social and Behavioral Sciences, 97*, 224 – 228.

Hameed, H., Hackling, M. W., & Garnett, P. J. (1993). Facilitating Conceptual Change in Chemical Equilibrium Using a CAI Strategy. *International Journal of Science Education, 15*, 221-230.

Hazzan, O. (1999). Reducing Abstraction Level When Learning Abstract Algebra Concepts. *Educational Studies in Mathematics, 40*, 71–90.

Healy, J. (2004). *Your Child's Growing Mind: Brain Development and Learning from Birth to Adolescence.* (3rd ed.). New York: Random House Inc.

Hicks, R. (1907). *Aristotle De Anima.* Cambridge: Cambridge University Press.

Hoffmann, R. (1995). *The Same and Not the Same* (Vol. XVI). New York: Columbia University Press.

Hoffmann, R., & Laszlo, P. (1991). Representation in Chemistry. *Angewandte Chemie, 30*, 1-16.

Horstmann, A. (1873, 2009). The Theory of Dissociation. *Annalen der Chemie und Pharmacie, Re-edited Bulletin for the History of Chemistry, 34*, 170,192-210.

Huddle, B. P. (1998). "Conceptual Questions" on Le Chatelier's Principle. *Journal of Chemical Education, 75,* 1175.

Huddle, P. A., White, M. W., & Rogers, F. (2000). Simulations for Teaching Chemical Equilibrium. *Journal of Chemical Education, 77*, 920-926.

Inhelder, B., & Piaget, J. (1958). *The Growth of Logical Thinking from Childhood to Adolescence.* London: Routledge & Kegan Paul.

Jensen, W. B. (1998). Logic, History, and the Chemistry Textbook: I. Does Chemistry Have a Logical Structure? *Journal of Chemical Education, 75,* 679–687.

Jensen, W. B. (2005). The Symbolism of Chemical Equations. *Journal of Chemical Education, 82,* 1461.

Jensen, W. B. (2009). August Horstmann and the Origins of Chemical Thermodynamics. *Bulletin for the History of Chemistry, 34*, 83-91.

Johnstone, A. H. (1982). Macro and Microchemistry. *School Science Review, 64*, 377-379.

Johnstone, A. H. (1991). Why is Science Difficult to Learn? Things are Seldom what they Seem. *Journal of Computer Assisted Learning, 7*, 75-83.

Johnstone, A. H. (1997). Chemistry Teaching - Science or Alchemy? *Journal of Chemical Education, 74,* 262-268.

Johnstone, A. H. (2000). Teaching of chemistry - Logical or Psychological? *Chemistry Education Research and Practice, 1*, 9-15.

Karpudewan, M., Treagust, D., Mocerino, M., Won, M., & Chandrasegaran, A. (2015). Investigating High School Students' Understanding of Chemical Equilibrium Concepts. *International Journal of Environmental & Science Education, 10,* 845-863.

Khan, S. (2011). New Pedagogies on Teaching Science with Computer Simulations. *Journal of Science Education and Technology, 20*, 215-232.

Knox, K. (1985). Le Chatelier's Principle. *Journal of Chemical Education, 62*, 863.

Kohlbacher, F. (2006). The Use of Qualitative Content Analysis in Case Study Research. *Qualitative Research, 7,* 1-30.

Kousathana, M., & Tsaparlis, G. (2002). Students' Errors in Solving Numerical Chemical-Equilibrium Problems. *Chemistry Education Research and Practice, 3*, 5-17.

Lakoff, G., & Johnson, M. (1980). The Metaphorical Structure of the Human Conceptual System. *Cognitive Science, 4*, 195-208.

Lakshminarayanan, A. (2010). Arrows in Chemistry. *Resonance, 15*, 51-63.

Lang, M. (2007). *Aspects of Boundary Crossing in Education. Summaries and Sources of Selected Literature Compiled for the CROSSNET Project.* Retrieved May 25, 2010, from CROSSNET: http://www.crossnet.uni-kiel.de/cms/index.php?id=3

Laurence, S., & Margolis, E. (2012). Abstraction and the Origin of General Ideas. *Philosophers' Imprint, 12*, 1-22.

Liu, H., Andre, T., & Greenbowe, T. (2008). The Impact of Learner's Prior Knowledge on Their Use of Chemistry Computer Simulations: A Case Study. *Journal of Science Education and Technology, 17*, 466-482.

Lower, S. (2001). *Chemical Equilibrium.* Retrieved March 05, 2004, from Simon Fraser University: http://www.sfu.ca/person/lower/Chem1Text/equilibrium/.

Lucena, A. D. (2005). *Filosofía de la ciência.* Madrid: Editorial Biblioteca Nueva.

MacDonald, J. (1976). *Chemical Equilibrium and its Conceptual Difficulties. MSc(R) Thesis.* Glasgow University.

Mahaffy, P. (2004). The Future Shape of Chemistry Education. *Chemistry Education Research and Practice, 5*, 229–245.

Martínez, S. F., & Huang, X. (2011). Epistemic Groundings of Abstraction and Their Cognitive Dimension. *Journal of the Philosophy of Science, 78,* 490-511 .

Martins, I., Costa, J., Lopes, J., Simões, M., Simões, T., Bello, A., et al. (2003). *Programa de Física e Química A – 11º ano – Curso Científico-Humanístico de Ciências e Tecnologias.* Lisboa: Ministério da Educação.

Maskill, R., & Cachapuz, A. F. (1989). Learning About Chemistry Topic of Equilibrium: the Use of Word Association Tests to Detect Developing Conceptualizations. *International Journal of Science Education, 11,* 57-69.

Matthews, M. (2002). Constructivism and Science Education: A Further Appraisal. *Journal of Science Education and Technology, 11,* 121-134.

Mayring, P. (2000). Qualitative Content Analysis. *Forum: Qualitative Social Research, 1.*

McLean, F. C. (1938). Application of the Law of Chemical Equilibrium (law of Mass Action) to Biological Problems. *Physiological Reviews, 18,* 495-523.

Meijer, M. (2011). *Macro-Meso-Micro Thinking with Structure-property Relations for Chemistry Education—an Explorative Design-based Study.* Utrecht: Utrecht University.

Mintzes, J. J., Wandersee, J. H., & Novak, J. D. (1998). *Teaching Science for Understanding. A Human Constructivist View.* San Diego: Academic Press.

Nacheva-Skopalik, L., & Koleva, M. (2012). Teaching Chemistry at Technical University. *Chemistry: Bulgarian Journal of Science Education, 24*, 176-186.

Nakhleh, M., & Mitchell, R. (1993). Concept Learning versus Problem Solving, There Is a Difference. *Journal of Chemical Education, 70*, 190-192.

Nature Chemistry. (2009). Editorial: Questioning "Chemistry". *Nature Chemistry, 1*, 671.

Niaz, M. (1995). Lakatosian Conceptual Change Teaching Strategy Based on Student Ability to Build Models with Varying Degrees of Conceptual Understanding of Chemical Equilibrium. *68th Anual Confrence of National Association for Research in Science Teaching.* San Francisco.

Niaz, M. (1998). From Cathode Rays To Alpha Particles To Quantum of Action: A Rational Reconstruction of Structure of the Atom and Its Implications for Chemistry Textbooks. *Science Education, 82*, 527-552.

Nicolopoulou, A. (1993). Play, Cognitive Development, and the SocialWorld: Piaget, Vygotsky, and Beyond. *Human Development, 36*, 1-23.

Ohlsson, S., & Lehtinen, E. (1997). Abstraction and the Acquisition of Complex Ideas. *International Journal of Educational Research, 27*, 37-48.

Oki, M. (2007). O Congresso de Karlsruhe e a Busca de Consenso Sobre a Realidade Atômica no Século XIX. *Química Nova na Escola, 26*, 24-28.

Olson, J., & Hansen, K. (2012). New Directions in Science Education and the Culture of the School – The CROSSNET Project as a Transnational Framework for Research. In K. Hansen, W. Gräber, & M. Lang (Eds.), *CROSSNET - Crossing Boundaries in Science Teacher Education* (p. 135−160). Munster: Waxmann.

Özmen, H. (2008). Determination of Students' Alternative Conceptions about Chemical Equilibrium: a Review of Research and the Case of Turkey. *Chemistry Education Research and Practice, 9*, 225–233.

Özmen, H. (2011). Turkish Primary Students' Conceptions about the Particulate Nature of Matter. *International Journal of Environmental & Science Education, 6*, 99-121.

Paiva, J. (2007). *O Fascínio de ser Professor.* Lisboa: Texto Editores.

Paiva, J. C., & Costa, L. (2010). Exploration Guides as a Strategy to Improve the Effectiveness of Educational Software in Chemistry. *Journal of Chemical Education, 87,* 589–591.

Paiva, J. C., Gil, V. M., & Correia, A. F. (2002). Le Chat: Simulation in Chemical Equilibrium. *Journal of Chemical Education, 79,* 640.

Paiva, J., & Fonseca, S. (2009). The Challenges of Using ICT to Cross Boundaries in the Teaching of Chemical Equilibrium – Portuguese Participation in CROSSNET. *Contemporary Science Education Research: Teaching* (pp. 269-272). Ankara: Pegem Akademi.

Paiva, J., & Fonseca, S. (2012). Facing Barriers in Teaching Chemical Equilibrium – Approahes based on the use of ICT. In K. Hansen, W. Gräber, & M. & Lang (Eds.), *Crossnet - Crossing Boundaries in Science Teacher Education* (p. 135−160). Münster: Waxman.

Paiva, J., Gonçalves, J., & and Fonseca, S. (2008). Does the Addition of Inert Gases, at Constant Volume and Temperature, affect Chemical Equilibrium? *Journal of Chemical Education, 85,* 1133-1135.

Partington, J. R. (1937). *A Short History of Chemistry.* New York: The Macmillan Company.

Pedrosa, M. A., & Dias, M. H. (2000). Chemistry Textbook Aproaches to Chemical Equilibrium and Student Alternative Conceptions. *Chemistry Education: Research and Practice in Europe, 1,* 227-236.

Pinto, M. L. (2002). *Práticas Educativas numa Sociedade Global.* Porto: Edições ASA.

Ponte, J. P. (2006). Estudos de Caso em Educação Matemática. *Bolema, 25,* 105-132.

Potgieter, M., Harding, A., & Engelbrecht, J. (2008). Transfer of Algebraic and Graphical Thinking between Mathematics and Chemistry. *Journal of Research in Science Teaching, 45,* 197–218.

Quílez, J. (2004). A Historical Approach to the Development of Chemical Equilibrium through the Evolution of the Affinity Concept: some Educational Suggestions. *Chemistry Education Research and Practice, 5,* 69-87.

Quílez, J. (2008). Theories in the Evolution of Chemical Equilibrium. *The 6th International Conference on the History of Chemistry - Neighbours and Territories: The Evolving Identity of Chemistry* (p. 695). Louvain-la-neuve: Mémosciences.

Quílez, J. (2009). From Chemical Forces to Chemical Rates: A Historical/Philosophical Foundation for the Teaching of Chemical Equilibrium. *Science & Education, 18*, 1203-1251.

Radder, H. (2006). *The World Observed/The World Conceived.* Pittsburgh: University of Pittsburgh Press.

Reger, D., Goode, S., & Mercer, E. (1997). *Química. Princípios e Aplicações.* (1ª, Ed.) Lisboa: Fundação Calouste Gulbenkian.

Renzi, S., & Klobas, J. (2000). Steps Toward Computer-supported Collaborative Learning for Large Classes. *Educational Technology & Society, 3*, 317-328.

Rol, M. E. (2007). *Conceptual Progress in Economics. Abstraction of Social Kinds versus Idealization.* Retrieved May 23, 2017, from http://www.rug.nl/research/portal/files/10206493/00a_introduction.pdf

Rosa, L. M. (2000). *A Integração das T.I.C. na Escola: Desafios, Condições e outras Reflexões.* Retrieved Janeiro 25, 2004, from Ágora: http://www.prof2000.pt/prof2000/agora3/agora3_4.html

Rosch, E. (1978). Principles of Categorization. In E. Rosch, & B. B. Lloy (Eds.), *Cognition and Categorization* (pp. 27-48). Hillsdale: Erlbaum.

Russell, J. M. (1988). Simple Models for Teaching Equilibrium and Le Chatelier's Principle. *Journal of Chemical Education, 65*, 871-872.

Russell, J. W., Kosma, R. B., Jones, T. W., Marx, N., & Davis, J. (1997). Use of Simultaneous-synchronized Macroscopic, Microscopic, and Symbolic Representations to Enhance the Teaching and Learning of Chemical Concepts. *Journal of Chemical Education, 74*, 330-334.

Sandberg, M., & Bellamy, M. K. (2003). Equilibrium. *Journal of Chemical Education, 80*, 456.

Sariçayir, H., Sahin, M., & Üce, M. (2006). Dynamic Equilibrium Explained Using the Computer. *Eurasia Journal of Mathematics, Science and Technology Education, 2*, 130-137.

Sawyer, D. J., & Martens, T. E. (1992). An Equilibrium Machine. *Journal of Chemical Education, 69*, 551-553.

Sebesta, R. (2012). *Concepts of Programming Languages* (10th ed.). New Jersey: Pearson.

Sinka, R. (2006). Primary School Teachers in the Information Society. *Journal of Universal Computer Science, 12*, 1358-1372.

Sirhan, G. (2007). Learning Difficulties in Chemistry: An Overview. *Journal of Turkish Science Education, 4*, 2–20.

Sirhan, G., Gray, C., Johnstone, A., & Reid, N. (1999). Preparing the Mind of the Learner. *University Chemistry Education, 3*, 43-46.

Sjöström, J. (2007). The Discourse of Chemistry (and Beyond). *HYLE – International Journal for Philosophy of Chemistry, 13*, 83-97.

Snead, L. P. (2011). *Difficulties Teaching Abstract Concepts in Secondary Chemistry Classroom.* Retrieved May 21, 2017, from http://www.ibrarian.net/navon/page.jsp?paperid=17617863&searchTerm=snead

Solaz, J. J., & Quílez, J. (2001). Changes of Extent of Reaction in Open Chemical Equilbria. *Chemistry Education Research and Practice in Europe, 2*, 303-312.

Sprague, D., Trey, S., Pillay, S., & Khan, S. (2005). How Computer Simulations Can Assist Model Generation in Students: Providing an Adaptable Structure to Guide Student Learning. In P. Richards, & G. Kommers (Eds), *Proceedings of World Conference on Educational Multimedia, Hypermedia and Telecommunications* (pp. 1666-1673). Montreal: Chesapeake.

Stieff, M., Ryub, M., & Yip, J. C. (2013). Speaking Across Levels – Generating and Addressing Levels Confusion in Discourse. *Chemistry Education Research and Practice, 13*, 376-389.

Stull, A. T., Hegarty, M., Dixon, B., & Stieff, M. (2012). Representational Translation With Concrete Models in Organic Chemistry. *Cognition and Instruction, 30*, 404-434.

Taber, K. S. (2001). Building the Structural Concepts of Chemistry: Some Considerations from Educational Research. *Chemistry Education Research and Practice in Europe, 2*, 123-158.

Taber, K. S. (2002). *Chemical Misconceptions - Prevention, Diagnosis and Cure: Theoretical Background.* London: Royal Society of Chemistry.

Taber, K. S. (2013). Revisiting the Chemistry Triplet: Drawing upon the Nature of Chemical Knowledge and the Psychology of Learning to Inform Chemistry Education. *Chemistry Education Research and Practice, 14*, 156-168.

Talanquer, V. (2011). Macro, Submicro, and Symbolic? The Many Faces of the Chemistry Triplet. *International Journal of Science Education, 33*, 179-195.

Thims, L. (2007). *Human Chemistry.* Morrisville: LuLu, Inc.

Thornton, C. (2003). Quantitative Abstraction Theory. *Journal of Artificial Intelligence and Simulation of Behaviour, 1*, 281-290.

Treptow, R. S. (1980). Le Chatelier principle. *Journal of Chemical Education, 57,* 417-420.

Tsaparlis, G. (1997). Atomic and Molecular Structure in Chemical Education – A Critical Analysis from Various Perspectives of Science Education. *Journal of Chemical Education, 74,* 923-925.

Tsaparlis, G. (2001). Preface Molecules and Atoms at the Centre Stage. *Chemistry Education Research and Practice in Europe, 2*, 57-65.

Tuomi-Grohn, T., & Engeström, Y. (2003). *Between School and Work: New Perspectives on Transfer and Boundary-Crossing.* Amsterdam: Pergamon.

Tyson, L., Treagust, D. F., & Bucat, R. B. (1999). The Complexity of Teaching and Learning Chemical Equilibrium. *Journal of Chemical Education, 76,* 554-558.

Van Driel, J. H., & Gräber, W. (2002). The Teaching and Learning of Chemical Equilibrium. In J. Gilbert, O. De Jong, R. Justi, D. Treagust, & J. Van Driel (Eds.), *Chemical Education: Towards Research-based Practice.* Dordrecht: Kluwer Academic Publishers.

Van Driel, J. H., De Vos, W., & Verloop, N. (1999). Introducing Dynamic Equilibrium as an Explanatory Model. *Journal of Chemical Education, 76*, 559-561.

Van't Hoff, J. H. (1901). Nobel Lecture, Osmotic Pressure and Chemical Equilibrium. Amsterdam: Elsevier Publishing Company.

Videira, A. (1993). Algumas Observações Históricas e Epistemológicas Sobre o Conceito de Átomo Clássico. *Revista Brasileira de História da Ciência, 10*, 13-20.

Weigold, M., & Treise, D. (2004). Attracting Teen Surfers to Science Web Sites. *Public Understanding of Science, 13*, 229–248.

Weller, S. W. (1999). Napoleon Bonaparte, French scientists, Chemical Equilibrium, and Mass Action. *Bulletin for the History of Chemistry*, *24*, 61-65.

Wilson, A. H. (1998). Equilibrium: A Teaching/Learning Activity. *Journal of Chemical Education, 75*, 1176-1177.

Wu, M., Tseng, K., & Greenan, J. (2003). How Can Reasoning Skills be Improved? - An Experimental Study of the Effects of Reasoning Skills Curriculum on Reasoning Skills Development for Students in Postsecondary Technical Education Programs. *European Conference on Educational Research.* Hamburg.

Yakmaci-Guzel, B., & Adadan, E. (2013). Use of Multiple Representations in Developing Preservice Chemistry Teachers' Understanding of the Structure of Matter. *International Journal of Environmental and Science Education*, *8*, 109-130.

Yin, R. (1994). *Case study research: Design and methods* (2nd ed.). Beverly Hills: Sage Publishing.

Ylvisaker, M. (2006). Self-Coaching: A Context-Sensitive, Person-Centred Approach to Social Communication After Traumatic Brain Injury. *Neurogenic Communication Disorders*, *7*, 246-258.

Zemansky, M. W. (1968). *Heat and Thermodynamics* (5th ed.). New York: McGraw-Hill Book Company Inc.

Zhang, Y., & Wildemuth, B. (2005). Qualitative Analysis of Content. *Analysis*, *1*, 1-12.

APPENDIX 1

INFORMATION ABOUT THE SIMULATION

In all simulations there are some limitations and approximations. In our case, the following are defined:

1. In the microscopic representation we suppose that the molecules are all of the same size, and much bigger than in reality. The colour is attributed randomly for a better distinction between species. These approximations do not interfere with the purposes for the microscopic representation like visualising the effect of disturbance and the contrast between ideal and real systems through the use of different inert gas pressures.
2. The kinetics of reactions has not been a preoccupation in this simulation since it would increase the complexity of construction, not contributing in a significant manner to its major objectives. Since in this phase there is only one system available, the risk of wrong comparing velocity of reactions is not present. Nevertheless, the increase in reaction velocity with temperature is considered in the prototype.
3. The "zoom" presented during equilibrium state, has, above all, the function of illustrating the variations in system compositions according to the partial pressures in equilibrium and inert gas pressures, using a more familiar molecular representation. So, the question of effective collisions is not explored, since it would imply the consideration of intermediary steps in the mechanism of reaction.

4. For reasons associated to the construction of the simulation, the proportions of points (representing the species in reaction) may vary slightly in relation to the exact numerical proportions. Since this is only a small variation is not perceptible and so does not influence any interpretation.
5. In the productivity it is considered only the quantity of products produced face to the initial quantity of reagents (in the case of beginning the reaction from the reagents). The kinetic factor and other aspects that can influence economically have not been considered in this calculation.
6. For ideal systems the results and calculations are the ones predicted by the mathematical expressions usually defined in school manuals and in conformity with Le Chatelier's principle. The values of equilibrium constant were determined through the thermodynamic data in bibliography and the expressions used are accessible in numerical data section accessible in "lamp" button. The method used in the establishment and reestablishment of equilibrium consists in a progressive approximation of the partial pressures of each specie and consequently of the quotient of reaction to the values of equilibrium pressures and equilibrium constant.
7. For real systems, namely in what refers to inert gas addition, this simulation presents an innovation, being possible to verify that the results differ from the predicted to ideal systems. The process of approximation to equilibrium is similar to the one used in ideal systems but the expressions that do quantify it are different. One of the objectives of constructing this simulation was the illustration of the result from a mathematical complex process in a way suitable for application in teaching. So, we do not intend that medium level students in Chemistry take direct contact with the mathematical deduction, but that they could get the perception that for real systems the conclusions may diverge from the ones obtained in ideal systems.

8. The shift from ideal to real, that happens when inert gas pressure is elevated to 10 bar, was defined based on mathematical expressions. We adopted the designation of real system when the influence of inert gas attained a centesimal variation.

APPENDIX 2

Exploration guide

Chemical Equilibrium simulation

The challenge of industrial control

Goals

It is intended to explore an educational multimedia application, performing various tasks, in order to understand the concepts concerning Chemical Equilibrium, namely the establishment, disturbance and restoration of the equilibrium state.

Software / Aplicação multimédia

Multimedia application available online, "Chemical Equilibrium simulation", located at: http://nautilus.fis.uc.pt/cec/teses/susana_fonseca/

Introduction

You observe the environment that surrounds you and find that you are in a room equipped with several instruments of technically advanced appearance. The temperature inside this room is high and you can hear background noise from something similar to running reactors.

You wonder about the way you came here. However, the curiosity to know more about this interesting place erases the doubts and fears that you are feeling and you begin to investigate the space around. An advertising style panel on one of the walls catches your eye. In this panel, a car of modern lines is visible with the slogan: "The Automobile of the Future in the Present! Powered by hydrogen!"

Below it is an indicative graph of economic profits, entitled "Monthly productivity". Associating the information, you begin to realize that you are in an industrial hydrogen production facility. In the centre of the room you can see a screen, a variety of controls and an empty chair, waiting for the coordinator of the factory operation.

Surprised by this situation, you haven't yet noticed the badge you have on your chest. You can read your name and the identification: "Engine room technician. Function: control of the industrial production". Fortunately, you find that there is a guide on the table, certainly intended to help you in the task that was assigned to you. With the indestructible curiosity of any young person with a scientific spirit, you begin to follow the directions of the script.

Good job!

Exploration Guide

1 What is the equilibrium state? To control this process you first have to know the state around which the Chemical Equilibrium is based!

Actions

1. After entering into the simulation address, press "start".
2. Select the reaction in which the gas produced in this plant and press "OK".
3. To obtain information on the establishment of the equilibrium use the but💡 .
4. Use the simulation to observe the aspects related to Chemical Equilibrium. To do this, select the temperature, pressure and reagent / product conditions on the rotary knob. Follow the instructions that appear on the black panel at the bottom of the simulation.
Click "equilibrate" and watch the evolution of the reaction.
5. Draw up a succinct definition of equilibrium state and write it down.

☑ Answers/Conclusions	Reflection
	The concentration of products and reagents remains constant during equilibrium state? *Observe the system at microscopic level. Does the reaction stop when equilibrium state is attained?* *Does it become slower?* *The quantity of reagents and products must be equal during equilibrium?* 1

2 Does the temperature influence the establishment of the equilibrium state of this reaction? How?

Actions

1. Start by setting the initial conditions of temperature, pressure and reagents / products on the rotary knob. Choose the values that you prefer and register them below.
2. Press "equilibrate" to allow the gases to enter the system and the reaction to proceed.
3. Observe carefully what happens until the equilibrium is established and after the its establishment.
4. At this stage you can check information on how the temperature affects the steady state with the button 💡 which will be necessary to correctly predict what happens when you change the temperature.
5. Return to the rotary knob and change just the temperature in relation to the first "equilibration".
6. Then press "equilibrate" again and make a prediction about the direction in which the equilibrium will shift due to the change in temperature.
7. Press again "equilibrate" and observe what happens. Confirm in the background if your prediction was correct.
8. Conclude about question and register the values required in the table below.

Registrations

The reaction is : *Endotermic* ☐ *Exotermic* ☐	*1st equilibrium state* *T =* *K =* *Quantity of products:*	*2nd equilibrium state* *T =* *K =* *Quantity of reagents:*	*Direction of equilibrium displacement due to the change in temperature:*

☑ Answers/Conclusions	Reflection
	Observe the microscopic representation (zoom) at different temperatures. What can you say about the temperature effect on the reaction rate? *Higher rate means larger concentrations?*

3 Does the pressure influence the establishment of the equilibrium state of this reaction? How?

Actions

1. Restart the simulation by pressing "OK".
2. Carry out a study similar to the previous question but now just changing the pressure between the first and second states of equilibrium, in order to conclude how this factor influences equilibrium.

Registrations

Variation in the number of moles of gaseous species between reagents and products:	*1st equilibrium state* *P =* *K =* *Products quantity:*	*2nd equilibrium state* *P =* *K =* *Products quantity:*	*Direction of equilibrium displacement due to pressure change:*

☑ Answers/Conclusions	Reflection
	What influence would the pressure have on a reaction with different number of gaseous moles between reagents and products such as iodine dissociation?

4 Does initiating the reaction starting with the products or the reagents lead to different equilibrium states?

Actions

1. Restart the simulation by pressing "OK".
2. Choose the desired pressure and temperature conditions and initiate the reaction starting from the reactants. Record the equilibrium data in the space below.
3. Restart the simulation by pressing "OK".
4. Choose the same pressure and temperature conditions and start the reaction from the products. Record the equilibrium data in the space below.
5. Draws conclusions on the question pose.

Registrations		☑ Answers/Conclusions
Equilibrium obtained starting from the reagents *K =* *Products quantity:*	*Equilibrium obtained starting from the products* *K =* *Products quantity:*	

5 How does the addition of a reagent influence the equilibrium state?

Actions

1. Restart the simulation by pressing "OK".
2. Choose the pressure and temperature conditions and reagents / products of your choice. Record the equilibrium data in the space below.
3. Add only reagent by selecting the reagents / products option on the rotary knob.
4. Press "equilibrate" and predict the shift of the equilibrium.
5. Press again "equilibrate", observe and record the values of the new equilibrium state.
6. Draw conclusions on the question pose.

Registrations			☑ Answers/Conclusions
1st equilibrium state *K =* *Products quantity:*	*2nd equilibrium state* *K =* *Products quantity:*	*Direction of equilibrium displacement due to the addition of reagent:*	

Reflection

Does the addition of reagents change the value of the equilibrium constant?

In the reestablished equilibrium, the quantity of reagents is higher or lower than in the first equilibrium?

6 Does the addition of inert gas affect equilibrium?

Actions

1. Restart the simulation by pressing "OK".
2. Choose the pressure and temperature conditions and reagents / products of your choice.
3. Add 1 bar of xenon by selecting the inert gas option on the rotary knob.
4. Check in the lower right corner of the main screen if the system is marked as ideal or real.
5. Press "equilibrate" and predict the direction of equilibrium shift.
6. Press again "equilibrate", observe and record data below.
7. Look closely at the microscopic representation of the system at equilibrium through the button
8. Go back to inert gas on the rotary knob and add 100 bar of xenon.
9. Check in the lower right corner of the main screen if the system is marked as ideal or real.
10. Press "equilibrate", make the prediction, press again "equilibrate" and observe what happens.
11. Record below the shift (if any) on the equilibrium.
12. Look closely at the microscopic representation of the system at equilibrium through the button
13. Draw conclusions on the question posed. You can always get more information at .

Registrations

Equilibrium shift by the addition of 1 bar of inert gas:	*Equilibrium shift by the addition of 100 bar of inert gas:*
1 bar of inert gas *Ideal System* ☐ *Real System* ☐	*100 bar of inert gas* *Ideal System* ☐ *Real System* ☐

☑ Answers/Conclusions

Now you should define the conditions of the system to obtain maximum productivity in the formation of hydrogen. Record the conditions chosen in the table below and explain briefly the options you took.

Go a little further and...

Explore the simulation deeper, creating various perturbations and combining different sets of conditions.

Use the section www , which has multiple websites related to Chemical Equilibrium and find out:

- why did Napoleon Bonaparte inadvertently contribute to the discovery of Chemical Equilibrium;
- who was Le Chatelier;
- the importance of the Haber process and the conditions to maximize its productivity.

Go to www.jogodascoisas.net and have fun testing your knowledge about Chemical Equilibrium.

Roteiro de Exploração

Simulação de Equilíbrio Químico

O Desafio do Controlo Industrial

Objectivos

Pretende-se explorar uma aplicação multimédia educativa, realizando diversas tarefas, com vista à compreensão do Equilíbrio Químico, no que respeita ao seu estabelecimento perturbação e restabelecimento.

Software / Aplicação multimédia

Aplicação multimedia disponível *on-line*, designada "Simulação de Equilíbrio Químico", situada no endereço: http://nautilus.fis.uc.pt/cec/ea/ na area de alunos.

Introdução

Observas o ambiente que te rodeia e verificas que te encontras numa divisão apetrechada de diversos equipamentos e de aparência tecnicamente avançada. A temperatura dentro desta sala é elevada e consegues ouvir um barulho de fundo de algo semelhante a reactores em funcionamento.

Interrogas-te sobre o modo como vieste aqui parar. Contudo, a curiosidade de saber mais sobre este interessante local, desvanece as dúvidas e receios que sentes e assim começas a investigar o espaço em redor. Um painel de estilo publicitário numa das paredes prende-te a atenção. Neste, é visível um automóvel de linhas modernas e o *slogan*: "O Automóvel do Futuro no Presente! Movido a Hidrogénio!"

Mais adiante, está um gráfico indicativo de lucros económicos, com o título: "Produtividade Mensal". Associando as informações, começas a perceber que te encontras numa unidade industrial de produção de hidrogénio. No centro da sala, avistas um ecrã, uma diversidade de comandos e uma cadeira vazia, que esperam o responsável pela coordenação do funcionamento da fábrica.

Distraído pelo meio e surpreendido com esta situação, só agora reparas no crachá que tens ao peito. Neste, podes ler o teu nome e a identificação: "Técnico(a) da sala de máquinas. Função: controlo da produção industrial". Felizmente, verificas que está um roteiro em cima da mesa, certamente destinado a ajudar-te nesta tarefa que te destinaram. Com a curiosidade indestrutível de qualquer jovem com espírito científico, começas a seguir as indicações do roteiro.

Bom trabalho!

Roteiro

1 O que é o estado de equilíbrio? Para controlares este processo primeiro tens de conhecer o estado em torno do qual se baseia a temática do Equilíbrio Químico!

Acções

1. Depois de te dirigires ao endereço da simulação, prime "iniciar".
2. Em seguida selecciona a reacção em que é produzido o gás comercializado nesta unidade industrial e prime "OK".
3. Para obteres informação sobre o estabelecimento do equilíbrio utiliza o botão 💡 .
4. Em seguida utiliza a simulação para observares os aspectos referentes ao Equilíbrio Químico que leste na informação. Para tal, selecciona as condições de temperatura, pressão e reagentes/produtos no botão rotativo. Vai seguindo as instruções que aparecem no painel negro no fundo da simulação. Prime "equilibrar" e fica atento à evolução da reacção.
5. Elabora uma definição sucinta de estado de equilíbrio e escreve-a abaixo.

Respostas/Conclusões	Reflexões
	As concentrações de produtos e reagentes mantêm-se constantes durante o estado de equilíbrio? *Observa o sistema a nível microscópico. A reacção pára ao atingir o equilíbrio?* *Torna-se mais lenta no equilíbrio?* 1 *A quantidade reagentes e produtos tem de ser igual no equilíbrio?*

2 Será que a temperatura influencia o estabelecimento do estado de equilíbro desta reacção? De que forma?

Acções

1. Começa por definir as condições iniciais de temperatura, pressão e reagentes/produtos no botão rotativo. Escolhe os valores que preferires e regista-os abaixo.
2. Pressiona "equilibrar" para permitires que os gases entrem no sistema e a reacção se processe.
3. Observa atentamente o que acontece até se estabelecer o equilíbrio e após o estabelecimento do mesmo.
4. Nesta fase podes consultar informação sobre o modo como a temperatura afecta o estado de equilíbrio no botão 💡 , que será necessária para preveres correctamente o que ocorre quando alterares a temperatura.
5. Regressa ao botão rotativo e altera apenas a temperatura em relação ao primeiro ensaio.
6. Em seguida prime "equilibrar" e efectua a previsão sobre o sentido em que o equilíbrio se irá deslocar devido à alteração da temperatura.
7. Prime novamente "equilibrar" e observa o que acontece. Confirma no painel de fundo se a tua previsão estava correcta.
8. Conclui acerca da questão colocada e regista no quadro abaixo.

Registos

A reacção é : *Endotérmica* ☐ *Exotérmica* ☐	*1º estado de equilíbrio* *T =* *K =* *Quantidade de Produtos:*	*2º estado de equilíbrio* *T =* *K =* *Quantidade de Produtos:*	*Sentido de deslocamento do equilíbrio em função da alteração de temperatura:*

Respostas/Conclusões

Reflexão

Observa a representação microscópica (na lupa) a diferentes temperaturas. O que podes dizer relativamente ao efeito da temperatura sobre a velocidade da reacção?

Maior velocidade traduz-se em maior concentração?

3 Será que a pressão influencia o estabelecimento do estado de equilíbrio desta reacção? De que forma?

Acções

1. Reinicia a simulação pressionando "OK".
2. Efectua um estudo semelhante ao da questão anterior mas agora alterando apenas a pressão entre o primeiro e o segundo estados de equilíbrio, de forma a concluíres de que modo esta influencia o mesmo.

Registos

Variação do número de moles de espécies gasosas entre reagentes e produtos:	*1º estado de equilíbrio* *P =* *K =* *Quantidade de Produtos:*	*2º estado de equilíbrio* *P =* *K =* *Quantidade de Produtos:*	*Sentido de deslocamento do equilíbrio em função da alteração de pressão:*

Respostas/Conclusões

Reflexão

Que influência teria a pressão numa reacção com variação do número de moles de espécies gasosas entre reagentes e produtos como a dissociação do iodo?

2

4 Será que iniciar a reacção pelos produtos ou pelos reagentes leva à obtenção de estados de equilíbrio diferentes?

Acções

1. Reinicia a simulação pressionando "OK".
2. Escolhe as condições de pressão e temperatura que preferires e inicia a reacção partindo dos reagentes. Regista os dados relativos ao equilíbrio estabelecido no espaço abaixo.
3. Reinicia a simulação pressionando "OK".
4. Escolhe as condições de pressão e temperatura iguais às que seleccionaste no ensaio anterior e inicia a reacção partindo dos produtos. Regista os dados relativos ao equilíbrio estabelecido no espaço abaixo.
5. Retira conclusões em relação à questão colocada.

Registos

Equilíbrio obtido partindo dos reagentes *K =* *Quantidade de Produtos:*	*Equilíbrio obtido partindo dos produtos* *K =* *Quantidade de Produtos:*

☑ Respostas/Conclusões

5 De que forma a adição de um reagente influencia o estado de equilíbrio?

Acções

1. Reinicia a simulação pressionando "OK".
2. Escolhe as condições de pressão e temperatura e reagentes/produtos que preferires. Regista os dados relativos ao equilíbrio estabelecido no espaço abaixo.
3. Adiciona apenas reagente através da selecção da opção reagentes/produtos no botão rotativo.
4. Prime "equilibrar" e efectua a previsão do deslocamento do equilíbrio.
5. Prime novamente "equilibrar", observa e regista os valores no novo equilíbrio.
6. Retira conclusões em relação à questão colocada.

Registos

1º estado de equilíbrio *K =* *Quantidade de Produtos:*	*2º estado de equilíbrio* *K =* *Quantidade de Produtos:*	*Sentido de deslocamento do equilíbrio em função da adição de reagente:*

☑ Respostas/Conclusões

Reflexão

A adição de reagentes altera a constante de equilíbrio?

No reestabelecimento de equilíbrio a quantidade de reagente é superior ou inferior à do primeiro equilíbrio?

A adição de um gás inerte ao sistema afecta o equilíbrio?

6 Acções

1. Reinicia a simulação pressionando "OK".
2. Escolhe as condições de pressão e temperatura e reagentes/produtos que preferires.
3. Adiciona 1 bar de xénon através da selecção da opção gás inerte no botão rotativo.
4. Repara no canto inferior direito do "ecrã" principal se nestas condições o sistema é ideal ou real.
5. Prime "equilibrar" e efectua a previsão do deslocamento do equilíbrio.
6. Prime novamente "equilibrar", observa e regista abaixo sobre o deslocamento do equilíbrio.
7. Observa em pormenor a representação microscópica do sistema no equilíbrio através do botão
8. Vai novamente a gás inerte no botão rotativo e adiciona 100 bar de xénon.
9. Repara no canto inferior direito do "ecrã" principal se nestas condições o sistema é ideal ou real.
10. Prime "equilibrar", faz a previsão, prime novamente "equilibrar" e observa o que acontece.
11. Regista abaixo sobre o deslocamento do equilíbrio.
12. Observa em pormenor a representação microscópica do sistema no equilíbrio através do botão
13. Retira conclusões em relação à questão colocada. Podes sempre obter informação em .

Registos

Deslocamento do equilíbrio por adição de 1 bar de gás inerte:	*Deslocamento do equilíbrio por adição de 100 bar de gás inerte:*
1 bar de gás inerte *Sistema Ideal* ☐ *Sistema Real* ☐	*100 bar de gás inerte* *Sistema Ideal* ☐ *Sistema Real* ☐

Respostas/Conclusões

Agora define as condições do sistema para a obtenção de produtividade máxima na formação de hidrogénio. Regista as condições escolhidas no quadro abaixo e explica de forma sucinta as opções que tomaste.

Vai um pouco mais longe e ...

Explora a simulação mais profundamente, efectuando varias perturbações e combinando diferentes conjuntos de condições.

Utiliza a secção www *que tem múltiplos sites de Internet relacionados com Equilíbrio Químico para descobrir:*

- *porque é que Napoleão Bonaparte contribuiu inadvertidamente para a descoberta do Equilíbrio Químico;*
- *quem foi Le Chatelier;*
- *a importância do processo Haber e as condições que estão em jogo para que a sua produtividade seja máxima.*

Vai www.jogodascoisas.net e diverte-te a testar o teu domínio do Equilíbrio Químico

APPENDIX 3

Questionnaire A (pre-test)

N.º of identification _____

This questionnaire is anonymous, so the answers given in each question will not be part of the evaluation of the student. The objective of conducting this study is to improve the teaching / learning of this subject and to extend the knowledge / develop the reasoning of the students. Therefore, you should analyze all the questions very carefully and answer individually, in this sheet, using a blue or a black pen.

---

1. Check all the options that correctly complete the following sentence.

In the state of chemical equilibrium ...

☐ reaction products continue to form;
☐ the concentration of reactants and products remains constant over time;
☐ the reaction continues to occur but more slowly;
☐ reagents continue to form;
☐ the concentration of reagents and products varies but in equal proportion, ensuring the maintenance of equilibrium state;
☐ no reaction occurs during equilibrium.
☐ the characteristics obtained are different if the reaction is initiated by the reactants or by the products.

To achieve the state of chemical equilibrium ...

☐ The forward reaction must be completed, before the reaction in the reverse direction begins;
☐ The reaction has to proceed alternately in both directions;
☐ The reaction must be reversible.

It is not possible to reach the state of chemical equilibrium ...

☐ In a very extensive reaction which is practically complete;
☐ In an open system with gaseous components;
☐ In a reaction with a very small extension.

2. Consider Haber-Bosch process of production of ammonia at a certain temperature:

$$N_2\ (g) + 3H_2\ (g) \rightleftharpoons 2NH_3\ (g) \qquad Kc > 1$$

Which of the following hypotheses could correspond to the equilibrium composition for this system at this temperature.
Answer: ________

	$\|N_2\|$	$\|H_2\|$	$\|NH_3\|$
A	2 mol/dm^3	2 mol/dm^3	4 mol/dm^3
B	1 mol/dm^3	2 mol/dm^3	8 mol/dm^3
C	1 mol/dm^3	3 mol/dm^3	2 mol/dm^3

3. Consider the following chemical reaction:

$$\mathbf{A + B \rightleftharpoons C + D}$$

After establishing a state of chemical equilibrium for this reaction (equilibrium state 1), the system was disturbed by the addition of reagent **A**, and a new equilibrium state (equilibrium state 2) was subsequently reached.

3.1 Fill in the blank spaces in the table below with the words: **increase, decrease or equal**.

	|A|	|B|	|C|	|D|
Equilibrium state 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Variation in the moment of addition of reagent A				

3.2 Fill in the blank spaces in the table below with the expressions **"greater than at equilibrium 1", "lower than at equilibrium 1" or "equal to equilibrium 1"**.

	|A|	|B|	|C|	|D|
Equilibrium state 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Equilibrium state 2				

3.3 Explain your reasoning in question 3.2.

3.4 The equilibrium constant would be altered by this perturbation? ___________

4. Temperature is one of the factors affecting equilibrium state.

4.1 Complete the blank spaces.

For an exothermic reaction, after disturbing a system in chemical equilibrium with a rise in temperature, when a new equilibrium state is established, the rate of the direct reaction will be __________ than at the initial equilibrium and the rate of the inverse reaction will be __________ than at the initial equilibrium. The extent of the forward reaction will be __________.

4.2 Mark the following sentences as true or false.

☐ A rise in temperature promotes collisions between the particles, leading to increased reaction extent.

☐ Variations in temperature do not change the value of the equilibrium constant.

☐ The temperature affects the equilibrium constant of a chemical reaction shifting its equilibrium state, but does not cause variation of the concentration of reactants and products.

5. Comment on the following statements.

When the pressure of a system is increased the volume decreases and it tends to react according to Le Chatelier´s principle, increasing the volume and moving towards the largest number of gaseous moles.

The addition of an inert gas in an ideal systems, at constant volume and temperature, increases the total pressure and this change is minimized by the displacement in the direction with the smaller number of gaseous moles.

Questionário A(pré-teste)

N.º de identificação _____

Este questionário é anónimo, pelo que as respostas dadas em cada questão não serão objecto de avaliação do aluno. O objectivo da sua realização é melhorar o ensino / aprendizagem desta temática e alargar os conhecimentos / desenvolver o raciocínio dos alunos. Assim sendo, analisa todas as questões com muita atenção e reponde de forma individual, nesta folha, a caneta azul ou preta.

---

1. Assinala todas as opções que completam as frases seguintes de forma verdadeira.

No estado de equilíbrio químico…

☐ continuam a formar-se produtos da reacção;
☐ a concentração dos reagentes e dos produtos mantém-se sempre constante ao longo do tempo;
☐ a reacção continua a ocorrer mas de forma mais lenta;
☐ continuam a formar-se reagentes;
☐ a concentração de reagentes e produtos varia mas em igual proporção, garantindo a manutenção do estado de equilíbrio;
☐ não ocorre reacção durante o equilíbrio.
☐ as características obtidas são diferentes se a reacção se iniciar pelos reagentes ou pelos produtos da reacção.

Para que se atinja o estado de equilíbrio químico…

☐ a reacção no sentido directo tem de ser concluída, antes que a reacção no sentido inverso comece;
☐ a reacção tem decorrer de forma alternada nos dois sentidos;
☐ a reacção tem de ser reversível.

Não é possível atingir o estado de equilíbrio químico…

☐ numa reacção muito extensa que praticamente se completa;
☐ num sistema aberto com componentes gasosos;
☐ numa reacção com muito pouca extensão.

2. Considera o Processo Haber-Bosch de produção do Amoníaco a uma dada temperatura:

$$N_2\,(g) + 3H_2\,(g) \rightleftharpoons 2NH_3\,(g) \qquad Kc > 1$$

Qual das seguintes hipóteses poderia corresponder à composição de equilíbrio para este sistema, a esta temperatura. Resposta:________

	$\|N_2\|$	$\|H_2\|$	$\|NH_3\|$
A	2 mol/dm^3	2 mol/dm^3	4 mol/dm^3
B	1 mol/dm^3	2 mol/dm^3	8 mol/dm^3
.C	1 mol/dm^3	3 mol/dm^3	2 mol/dm^3

3. Considera a seguinte reacção química:

$$\mathbf{A + B \rightleftharpoons C + D}$$

Depois de estabelecido um estado de equilíbrio químico para esta reacção (Estado de Equilíbrio 1), este foi perturbado pela adição de uma dada quantidade do reagente **A**, sendo posteriormente atingido um novo estado de equilíbrio (Estado de Equilíbrio 2).

3.1 Completa os espaços em branco na tabela abaixo com as palavras: **aumenta, diminuiu ou mantém-se.**

	|A|	**|B|**	**|C|**	**|D|**
Estado de Equilíbrio 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Variação no momento da adição do reagente A.				

3.2 Completa os espaços em branco na tabela abaixo com as expressões: **“maior que no estado de equilíbrio 1” “menor que no estado de equilíbrio 1” ou “igual ao estado de equilíbrio 1”.**

	|A|	**|B|**	**|C|**	**|D|**
Estado de Equilíbrio 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Estado de Equilíbrio 2				

3.3 Explica o teu raciocínio na resposta à questão 3.2.

3.4 A constante de equilíbrio seria alterada por esta perturbação? ___________

4. A temperatura é um dos factores que afectam o estado de equilíbrio de um sistema reaccional.

4.1 Completa os espaços em branco.

Numa reacção exotérmica, depois de perturbar um sistema em equilíbrio químico com uma subida de temperatura, ao estabelecer-se um novo estado de equilíbrio, a velocidade da reacção directa será __________ que no equilíbrio inicial e a velocidade da reacção inversa será __________ que no equilíbrio inicial. A extensão da reacção no sentido directo será __________.

4.2 Assinala as frases seguintes com verdadeiro e falso.

☐ Uma subida da temperatura, promove as colisões entre as partículas, levando ao aumento da extensão da reacção.

☐ Variações de temperatura não alteram o valor da constante de equilíbrio.

☐ A temperatura afecta a constante de equilíbrio de uma reacção química perturbando o equilíbrio químico, mas não provoca variação da concentração de reagentes e produtos.

5. Comenta as afirmações seguintes.

Quando se aumenta a pressão de um sistema o volume diminui e este tende a reagir de acordo com o principio de Le Chatelier, aumentando o volume e deslocando-se no sentido do maior número de moles gasosas.

A adição de gás inerte em sistemas ideais, a volume e temperatura constantes, aumenta a pressão total e esta alteração é minimizada pelo deslocamento no sentido em que há diminuição do número de moles;

.

Questionnaire B (post-test)

N.º of identification _____

This questionnaire is anonymous, so the answers given in each question will not be part of the evaluation of the student. The objective of conducting this study is to improve the teaching / learning of this subject and to extend the knowledge / develop the reasoning of the students. Therefore, you should analyze all the questions very carefully and answer individually, in this sheet, using a blue or a black pen.

---

1. Check all the options that correctly complete the following sentence.

In the state of chemical equilibrium ...

☐ the concentration of reagents and products varies but in equal proportion, ensuring the maintenance of equilibrium state;
☐ the concentration of reactants and products remains constant over time;
☐ reaction products continue to form;
☐ the reaction continues to occur but more slowly;
☐ the characteristics obtained are different if the reaction is initiated by the reactants or by the products.

☐ no reaction occurs during equilibrium.
☐ reagents continue to form;

To achieve the state of chemical equilibrium ...

☐ The forward reaction must be completed, before the reaction in the reverse direction begins;
☐ The reaction must be reversible.
☐ The reaction has to proceed alternately in both directions;

It is not possible to reach the state of chemical equilibrium ...

☐ In a reaction with a very small extension.
☐ In a very extensive reaction which is practically complete;
☐ In an open system with gaseous components;

2. Consider Haber-Bosch process of production of ammonia at a certain temperature:

$$N_2\,(g) + 3H_2\,(g) \rightleftharpoons 2NH_3\,(g) \qquad Kc > 1$$

Which of the following hypotheses could correspond to the equilibrium composition for this system at this temperature.
Answer: ________

	$\lvert N_2 \rvert$	$\lvert H_2 \rvert$	$\lvert NH_3 \rvert$
A	1 mol/dm^3	2 mol/dm^3	8 mol/dm^3
B	2 mol/dm^3	2 mol/dm^3	4 mol/dm^3
C	1 mol/dm^3	3 mol/dm^3	2 mol/dm^3

3. Consider the following chemical reaction:

$$\mathbf{A + B \rightleftharpoons C + D}$$

After establishing a state of chemical equilibrium for this reaction (equilibrium state 1), the system was disturbed by the addition of **reagent B**, and a new equilibrium state (equilibrium state 2) was subsequently reached.

3.1 Fill in the blank spaces in the table below with the words: **increase, decrease or equal**.

	|A|	**|B|**	**|C|**	**|D|**
Equilibrium state 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Variation in the moment of addition of **reagent B**				

3.2 Fill in the blank spaces in the table below with the expressions **"greater than at equilibrium 1", "lower than at equilibrium 1" or "equal to equilibrium 1"**.

	|A|	**|B|**	**|C|**	**|D|**
Equilibrium state 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Equilibrium state 2				

3.3 Explain your reasoning in question 3.2.

3.4 The equilibrium constant would be altered by this perturbation? ___________

4. Temperature is one of the factors affecting equilibrium state.

4.1 Complete the blank spaces.

For an exothermic reaction, after disturbing a system in chemical equilibrium with a rise in temperature, when a new equilibrium state is established, the rate of the direct reaction will be __________ than at the initial equilibrium and the rate of the inverse reaction will be __________ than at the initial equilibrium. The extent of the forward reaction will be __________.

4.2 Mark the following sentences as true or false.

☐ Variations in temperature do not change the value of the equilibrium constant.
☐ A rise in temperature promotes collisions between the particles, leading to increased reaction extent.
☐ The temperature affects the equilibrium constant of a chemical reaction shifting its equilibrium state, but does not cause variation of the concentration of reactants and products.

5. Comment on the following statements.

When the pressure of a system is increased the volume decreases and it tends to react according to Le Chatelier´s principle, increasing the volume and moving towards the largest number of gaseous moles.

The addition of an inert gas in an ideal systems, at constant volume and temperature, increases the total pressure and this change is minimized by the displacement in the direction with the smaller number of gaseous moles.

Questionário B (pós-teste)

N.º de identificação _____

Este questionário é anónimo, pelo que as respostas dadas em cada questão não serão objecto de avaliação do aluno. O objectivo da sua realização é melhorar o ensino / aprendizagem desta temática e alargar os conhecimentos / desenvolver o raciocínio dos alunos. Assim sendo, analisa todas as questões com muita atenção e reponde de forma individual, nesta folha, a caneta azul ou preta.

---

1. Assinala todas as opções que completam as frases seguintes de forma verdadeira.

No estado de equilíbrio químico…

☐ a concentração de reagentes e produtos varia mas em igual proporção, garantindo a manutenção do estado de equilíbrio;

☐ a concentração dos reagentes e dos produtos mantém-se sempre constante ao longo do tempo;

☐ continuam a formar-se produtos da reacção;

☐ a reacção continua a ocorrer mas de forma mais lenta;

☐ as características obtidas são diferentes se a reacção se iniciar pelos reagentes ou pelos produtos da reacção.

☐ não ocorre reacção durante o equilíbrio.

☐ continuam a formar-se reagentes;

Para que se atinja o estado de equilíbrio químico…

☐ a reacção no sentido directo tem de ser concluída, antes que a reacção no sentido inverso comece;

☐ a reacção tem de ser reversível.

☐ a reacção tem decorrer de forma alternada nos dois sentidos;

Não é possível atingir o estado de equilíbrio químico…

☐ numa reacção com muito pouca extensão.

☐ numa reacção muito extensa que praticamente se completa;

☐ num sistema aberto com componentes gasosos;

2. Considera o Processo Haber-Bosch de produção do Amoníaco a uma dada temperatura:

$$N_2\,(g) + 3H_2\,(g) \rightleftharpoons 2NH_3\,(g) \qquad K\text{c} > 1$$

Qual das seguintes hipóteses poderia corresponder à composição de equilíbrio para este sistema, a esta temperatura. Resposta:________

	$\lvert N_2 \rvert$	$\lvert H_2 \rvert$	$\lvert NH_3 \rvert$
A	1 mol/dm^3	2 mol/dm^3	8 mol/dm^3
B	2 mol/dm^3	2 mol/dm^3	4 mol/dm^3
.C	1 mol/dm^3	3 mol/dm^3	2 mol/dm^3

3. Considera a seguinte reacção química:

$$\mathbf{A + B \rightleftharpoons C + D}$$

Depois de estabelecido um estado de equilíbrio químico para esta reacção (Estado de Equilíbrio 1), este foi perturbado pela adição de uma dada quantidade do **reagente B**, sendo posteriormente atingido um novo estado de equilíbrio (Estado de Equilíbrio 2).

3.1 Completa os espaços em branco na tabela abaixo com as palavras: **aumenta, diminuiu ou mantém-se.**

	|A|	**|B|**	**|C|**	**|D|**
Estado de Equilíbrio 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Variação no momento da adição do **reagente B.**				

3.2 Completa os espaços em branco na tabela abaixo com as expressões: **“maior que no estado de equilíbrio 1” “menor que no estado de equilíbrio 1” ou “igual ao estado de equilíbrio 1”.**

	|A|	**|B|**	**|C|**	**|D|**
Estado de Equilíbrio 1	**2 mol/dm^3**	**3 mol/dm^3**	**2 mol/dm^3**	**2 mol/dm^3**
Estado de Equilíbrio 2				

3.3 Explica o teu raciocínio na resposta à questão 3.2.

3.4 A constante de equilíbrio seria alterada por esta perturbação? ___________

4. A temperatura é um dos factores que afectam o estado de equilíbrio de um sistema reaccional.

4.1 Completa os espaços em branco.

Numa reacção exotérmica, depois de perturbar um sistema em equilíbrio químico com uma subida de temperatura, ao estabelecer-se um novo estado de equilíbrio, a velocidade da reacção directa será __________ que no equilíbrio inicial e a velocidade da reacção inversa será __________ que no equilíbrio inicial. A extensão da reacção no sentido directo será __________.

4.2 Assinala as frases seguintes com verdadeiro e falso.

☐ Variações de temperatura não alteram o valor da constante de equilíbrio.

☐ Uma subida da temperatura, promove as colisões entre as partículas, levando ao aumento da extensão da reacção.

☐ A temperatura afecta a constante de equilíbrio de uma reacção química perturbando o equilíbrio químico, mas não provoca variação da concentração de reagentes e produtos.

5. Comenta as afirmações seguintes.

Quando se aumenta a pressão de um sistema o volume diminui e este tende a reagir de acordo com o principio de Le Chatelier, aumentando o volume e deslocando-se no sentido do maior número de moles gasosas.

A adição de gás inerte em sistemas ideais, a volume e temperatura constantes, aumenta a pressão total e esta alteração é minimizada pelo deslocamento no sentido em que há diminuição do número de moles;