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Constructing a Novel E-Learning Course, Educational Computational Chemistry through Instructional Design Approach in the TPASK Framework

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Abstract: The educational scenario after the COVID-19 confinement presents new challenges for teachers. Technological advances require teachers to be prepared for instruction through technology, and with this, the need for e-learning courses arose to strengthen this knowledge. This article aims to describe an innovative e-learning course in Educational Computational Chemistry (ECC) for in-service chemistry teachers through an Instructional Design (ID) that allows the development of the constructs associated with the Technological Pedagogical Science Knowledge (TPASK) framework. From the literature overview, relevant findings were raised concerning ID and its potential technological support. The results indicate that an effective ID must present general elements, such as the organisation and generation of content, progress monitoring, and feedback instances. However, the stages of engagement, flexibility, and positioning are relevant elements. These design elements are linked to emerging technological tools, such as artificial intelligence for generating audiovisual material, interactive content development, and event logs. In addition, positive results are evident from the teachers who participated in the ECC e-learning course, who project the knowledge, computer skills, and learning acquired into their professional work as chemistry teachers. Based on the above, a course design for ECC is proposed with general guidelines that contribute to the continuous training of in-service chemistry teachers.

Keywords: instructional design; teacher professional development; in-service teachers training; ICT-enhanced learning; TPASK; online learning; e-learning

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1. Introduction

The current educational scenario demands competent chemistry teachers who innovate and develop the necessary skills to promote in their students the competencies that allow them to understand the natural and technological world to participate in an informed manner in the decisions and actions that affect their well-being and that of society [1]. In this regard, the continuous training of science teachers is fundamental since it allows for the updating and development of professional competencies that are indispensable for the constant improvement of educational practices in the sciences. Especially Technological Pedagogical Science Knowledge (TPASK) is needed, i.e., understanding how to use emerging science technology to implement learning environments that promote science

learning in students. There is a need to use a suitable Instructional Design (ID) approach [2] to construct e-learning courses for supporting teachers' work at the school level.

Incorporating Information and Communication Technologies (ICT) in the educational field has allowed innovation in didactic strategies, management, and administration of teaching and learning processes of the sciences [3,4]. Nowadays, technological advances and the Internet have made e-learning courses proliferate all over the world. These courses arise with the mission of achieving learning, improving the skills and abilities scientific of students, and enabling interactive, flexible learning with remote access without contemplating the physical space or specific hours as obstacles [5].

In this sense, the TPASK framework [6] shows how to use emerging science technology to implement learning environments that promote science learning in students. Said implementation becomes complex due to the particular needs of teachers. Helppolainen and Aksela [7] report that in-service teachers have limited progress in technology related to pedagogical and scientific aspects. In our previous research in chemistry teacher training, we have highlighted the need to integrate emerging scientific technologies in the design of chemistry teacher training of educational scenarios that promote Education for Sustainable Development (ESD) using socio-scientific issues (SSI) as a basis [8–10]. Due to the above, the Instructional Design (ID) of the e-learning course becomes fundamental since it contemplates the process of analysis, design, and development of the educational scenario. However, it is necessary to incorporate into the ID the aspects associated with the constructs present in the TPASK of in-service chemistry teachers since the current continuing education needs must respond to the post-pandemic educational requirements.

This study aims to describe an innovative e-learning course in ECC for in-service chemistry teachers through an ID that allows the development of the constructs associated with the TPASK.

The research questions are:

- RQ1. What are the elements or characteristics that an e-learning ID should consider for the development of TPASK in post-pandemic chemistry teachers?
- RQ2. How relevant is the ECC course designed through the ID approach for teachers?

In this article, firstly, we contextualise the importance of ID in learning environments, along with a theoretical framework behind the TPASK model, which is necessary to understand the design decisions involved in developing the ECC e-learning course. Then, the course is described, and finally, the perceptions of the participating in-service teachers are collected.

1.1. Instructional Design

There are different ID models in the literature, and they allow for connecting a learning theory with its immediate application. In this sense, the theoretical approach under which the instructional designer organises the teaching and learning process is evident. Historically, ID has been based on design models, from behavioural models in the 1960s to much more holistic models in the 1990s. These models generally incorporate systematised sequences to develop various training actions, which are widely documented in the Gagné and Briggs model [11], the Jonassen model [12], the Dick and Carey model [13], the ASSURE model (an acronym for Analyse learners, State objectives, Select media and materials, Utilise materials, Require learner participation, and Evaluate/revise) [14], and the ADDIE model (an acronym for Analyze, Design, Develop, Implement, and Evaluate) [15]. Although these models incorporate stages of analysis, development, and implementation, in practice, they may become inflexible, becoming a checklist to ensure the design of a learning environment.

In e-learning environments, ID is based on using ICT to support the generation of learning environments based on the use of technological tools for knowledge generation. In this line, we find the web-based e-learning model [16] and the instructional design for online learning (IDOL) model [17]. However, these models do not consider technology a dynamic component [18].

Chemistry teachers usually organise their time between school assignments and continuous training. In this sense, it is necessary to design e-learning courses structured using brief modules focusing on scientific topics relevant to the school environment [19]. Additionally, some studies highlighted the necessity of providing teachers with training on effectively utilising technological tools to enhance their pedagogical practices. This training is because teachers typically have a minimum academic background regarding digital technologies, and even less so in the context of chemistry education. Consequently, their use of digital technologies is not frequently incorporated into their pedagogical practices [20,21].

However, in the mid-2020s, education underwent a relevant change due to the global confinement resulting from COVID-19 and the call to keep educational processes ongoing in both schools and universities [22]. Teachers had to transform classical teaching into remote teaching to alleviate the situation. During this period, there has been a significant boom in the offer of massive open online courses (MOOCs) [23]. In addition, the use of free databases to learn about the latest advances and scientific discoveries related to COVID-19 is highlighted. Web-based chemical structure visualisation tools have also increased in importance, allowing for a more efficient understanding of symmetry, functionality, site of action, and chemical reactions [24,25].

Along with this, the urgency of implementing e-learning courses worldwide arose. With this, new pedagogical and didactic needs were revealed, such as emerging technologies and the sudden shift to fully online chemistry teaching [26].

Problem-Based Learning in the Framework of E-Learning Instructional Design

The implementation of educational environments based on ICT is favoured by implementing learning environments centred on the student, who becomes an active agent, the student is a participant in his educational process, and it is he who must learn to solve complex situations based on real, relevant and meaningful problems for citizenship [27,28]. In this sense, Problem-Based Learning (PBL) is positioned as a learning methodology with strong support on authentic, real problems as a starting point for acquiring and integrating new knowledge.

Our research group has researched the socio-scientific problems in PBL scenarios, generating evidence through perception studies with pre-service chemistry teachers that show that students develop their Science Knowledge (SK), Technological Science Knowledge (TSK), and canonical TPASK. These students projected using these technology-enriched scenarios in their future professional development [8–10]. In this regard, the socio-scientific problem in PBL technology-enriched scenario is an interesting design element for science e-learning courses oriented to in-service teachers. Additionally, the e-learning system provides the traditional PBL with greater interactive and multimedia resources, favour understanding the problem [29]. However, the ID of a course combining e-learning and PBL (e-PBL) should differ from that of a traditional approach. The ID is much more structured and oriented to use the resources effectively [30]. In standard PBL, the teacher is positioned as a constant monitor; on the contrary, in e-PBL, there is no guidance for each work team, but rather the teacher maintains an overview of the course, interacting mainly through the general forum. In this sense, Kim and Kee [30], in a mixed study of physicians in training who took 12 e-PBL modules, report that e-PBL promotes the development of autonomy and individual reasoning. Similarly, Setyani et al. [31], in a quantitative study with economics students, report that e-PBL significantly boosted students' motivation and attitude towards learning during the pandemic.

Due to the above, the ID that incorporates e-PBL as a development methodology together with emerging technological tools and socio-scientific problems is positioned as a way to implement e-learning courses that allow contributions to the development of teachers and students.

1.2. From Pedagogical Content Knowledge to Technological Pedagogical Science Knowledge

From the initial conceptions of professional teaching knowledge proposed by Shulman [32], the Pedagogical Content Knowledge (PCK) framework, understood as the re-elaboration of the knowledge of a discipline to be taught, is based on the interpretation of the content by the teacher and the various ways in which it can be represented.

Although this construct has had various interpretations [33,34], a framework for its analysis is the one proposed by Chen and Chen [35], who, studying the development of PCK of in-service chemistry teachers, report that this construct is consolidated from nine sources: (i) learning experience as a student in primary and secondary school; (ii) pre-service university training experience; (iii) in-service training experience, through continuing education programs, conferences, seminars or workshops organised by schools; (iv) classroom observations among peers; (v) peer coaching; (vi) self-instruction through reading professional journals on science/chemistry education; (vii) learning through online resources such as online training programs and teaching materials; (viii) personal self-reflection about teaching experience; and (ix) reading curricular materials such as textbooks and teachers' guides. Their findings show that chemistry teachers mainly develop their PCK from (i) personal teaching experience, (ii) reflection on their practices, (iii) classroom observation, and (iv) peer work. On the one hand, these findings are in agreement with what has been previously reported by Helms and Stokes [36], who report that every teacher has a personal PCK based on their teaching experience and, therefore, a teacher with more years of practice should have a more robust PCK than a teacher who has just started teaching [37]. Additionally, Chen and Chen [35] reveal the need to promote the continuous training of teachers in aspects related to practical work, which could be understood as the promotion of the canonical PCK, that is, a particular knowledge that can be shared and applied by many teachers [38,39].

In the last two decades, the Technological Pedagogical Content Knowledge (TPACK) framework formulated by Mishra and Koehler [40] has become very relevant in the academic community, based on integrating pedagogical and curricular knowledge teachers should have to use technology integrally in teaching. In other words, the TPACK model comprises the knowledge that teachers should have related to disciplinary content, pedagogy, and technology. Three new constructs emerge from the interrelations among these fundamental fields of knowledge: (i) Technological Content Knowledge (TCK), which is based on the integration between technology and content, understanding that through the use of technology, new representations of content can be generated; (ii) Technological Pedagogical Knowledge (TPK), which accounts for the modifications that teaching and learning processes can undergo when using particular technologies; and (iii) TPACK, which is the effective integration of technology in the teaching and learning process, making it possible to identify the knowledge necessary for the teacher to achieve this end in their educational practice [41–43].

To represent what science teachers need to know about technology to carry out a science teaching practice that adequately integrates technology, Jimoyiannis [6] proposes TPASK as an adaptation of the TPACK model and defines it as a type of knowledge specific to science teachers, different from the knowledge of a disciplinary expert (a physicist, chemist, or biologist), or a technology expert, and even from the general pedagogical knowledge shared by teachers of other disciplines. Based on our research and our team's experience in science teacher education, we support the perspective that TPASK should be understood as a distinct body of knowledge that can be developed from an integrative model. TPASK framework has seven constructs of knowledge, some of which have been adapted by our research team:

TK is how to use emerging technologies in a specific scientific domain.

SK represents understanding the scientific community's models, protocols, practices, and products in science [9].

PK is the general knowledge about learning and teaching.

PSK represents the understanding of models, protocols, practices, and products of the science fields included in science education and the knowledge used to implement learning environments that promote student learning. In addition, it consists of an understanding of students' construction of scientific knowledge in teaching contexts [9].

TSK represents the knowledge of using models and simulations to illustrate and apply scientific concepts using emerging technology, e.g., that linked to computational science [10].

TPK' is the knowledge about the possibilities and challenges involved in different ways of teaching and learning.

TPASK understands how to use emerging science technology to implement learning environments that promote science learning in students [10].

The TPASK framework linked to chemistry has been widely studied in teacher training and in-service teachers. From the initial training, the main findings indicate that integrating technology in training is long since teachers have difficulties relating technologies with instructional purposes [44,45]. In this sense, Cetin-Dindar et al. [46], through a quantitative study, show that by the use of didactic material generation courses incorporating technology during the training of 17 teachers, they did not present a significant increase in the development of their TSK and TPK'; instead, the teachers in training improved significantly in aspects related to PK and PSK.

Concerning in-service chemistry teachers, the main findings account for the technological tools incorporated in practice, such as interactive whiteboards [47], virtual laboratories and simulators [48,49], online blogs [50], social networks [51], and video clips [52,53] and its linkage with the TPK and TSK developments'. In other words, as technical support to teaching activities instead of a piece of fundamental knowledge in the design of their practices. Although the effective integration of technology should encourage teachers to perform student-centred activities, several authors indicate the need for further studies that reveal the importance of the use of technology for teaching and learning chemistry since the specific integration of technologies is still not visualised in the planning of teaching activities [8,45,54–56].

However, during the development of the COVID-19 pandemic and the resulting call for confinement, as well as the urgent need to organise education based on the use of technology, the knowledge bodies associated with TPASK among in-service chemistry teachers experienced a significant surge. In the first instance, teachers implemented a greater number and variety of technological tools in their practice, from synchronous teaching platforms (Zoom, Meet, MS Teams), asynchronous (Moodle, websites) to direct means of communication (WhatsApp, Telegram, Emails). These actions mainly account for TK and TPK' [57]. In agreement with Rap et al. [26], during the first stage of the pandemic, teachers paid little attention to TPASK since the urgency led teachers to use a more significant number of technological tools to transition from the traditional chemistry class to the online chemistry class.

During the second stage of the pandemic, mid-2020, there was evidence of a change in the perception of chemistry teachers towards distance learning. Although initially there was some fear on the part of teachers related to the lack of TK, the findings realise that teachers incorporated a greater amount of resources linked to online teaching, for example, the use of Learning Management Systems (LMS) complemented by the generation of interactive material using web tools as support; due to this, an improvement in digital skills and a strengthening of their TPK' were evidenced [58,59]. These elements are relevant as a starting point for an ID of chemistry e-learning courses oriented to in-service teachers.

During the third stage of the pandemic, mid-2021, gamification gained strength from chemistry, and various applications emerged that were incorporated into online teaching. According to the evidence, using games or challenges creates attractive learning environments for students. In this line appeared, for example, ChemiPuzzle [60], an interactive puzzle with a focus on aspects linked to Lewis structure, isomerism, and chemical bonds; Chemical escape rooms [61], a virtual environment based on atom knowledge, radioactiv-

ity, the periodic table; Zu Kon 2030 [62], a virtual scenario that uses sustainability from a chemical point of view and also introduces students to the SD Goals (SDGs) of the 2030 Agenda, and MedChemBlog [63], as an instance that invites students to elaborate blogs from information provided from chemical databases, such as Protein Data Bank [64] or PubChem [65]. In this sense, there is an incipient development of TSK by teachers. Several authors highlight the need to enhance the development of TSK to strengthen the TPASK of teachers [66,67] since a teacher who manages to position himself from a robust TPASK can select and use in his planning resources and scientific–technological tools that provide adequate support for teaching and learning of students.

Based on the above, this article shows an ID oriented to develop the constructs of TK, TPK', and TSK in post-pandemic chemistry teachers from an ECC e-learning course.

2. Materials and Methods

2.1. ID Elements and Proposal for the Generation of an ECC E-Learning Course

The literature overview of the current ID models linked to teachers' professional development was developed to fulfil this study's objective, based on courses related to e-learning chemical education. In addition, it was collected information on LMS and technological tools that allow the development of the ID process, linked to the generation of content (videos, activities, evaluations, surveys) as well as the form of implementation of the educational scenario. In this sense, the purpose is to gather updated and relevant information on the ID used. For this purpose, we consulted original articles and reviews from the Web of Science main collection over the last five years. The papers that report on the ID of e-learning courses related to science or chemistry and show its constituent elements were used as search criteria.

Based on the analysis of the reported findings and the current needs of in-service chemistry teachers reported in post-pandemic research, the design of an ECC course within the TPASK framework is proposed.

2.2. Perception of In-Service Chemistry Teachers Participating in the ECC E-Learning Course

The study population comprised 108 in-service teachers participating in the ECC e-learning course, characterised using a survey identifying computational chemistry elements (see the survey in Table S1). The focus group sample's selection criteria were as follows:

(i) Participants with more than three years of teaching experience (i.e., those who were actively teaching during the pandemic);
(ii) Participants with limited knowledge of computational chemistry elements;
(iii) Participants who had completed at least 90% of the proposed course activities.

Finally, the focal group comprised six teachers, who were identified using a code (Id_i; i = 1–6) in consideration of the guidelines delivered by the Ethics Committee.

The focus group gave us the perception of in-service chemistry teachers participating in the ECC e-learning. This focus was conducted synchronic using an open questionnaire (Table S2). An external moderator led the focus group. The session was recorded on video and transcribed to ensure the accuracy of the generated information. Data analysis was performed using qualitative content analysis [68], categorising the participants' expressions based on the following categories related to instructional design (ID):

(i) Experience with the virtual environment of the ECC e-learning course;
(ii) Facilitators for learning chemistry and science in general;
(iii) Computational chemistry or Cheminformatics: uses, knowledge, and skills;
(iv) Generation of a PBL environment and projections in their teaching work.

The validity and reliability were established based on the proposals of previous research on chemistry teacher education [9,10].

3. Results

3.1. ID for ECC E-Learning Course (RQ1)

From the literature overview of the ID models [11–17,69], which were included in the supplementary information (Table S3), seven relevant elements emerge for generating effective learning environments in the current technological reality (Table 1).

Table 1. Relevant elements to generating effective learning environments mediated by technology.

Element	Description
LMS	The platform to be used must give the proper support to the course, with a friendly interface that allows intuitive navigation that facilitates the search for information and the completion of tasks.
Learning Goals	The learning objectives in an e-learning course must be clear, specific, and achievable for the students. These objectives must be designed so that students clearly understand what is expected of them and what they are expected to achieve by the end of the course.
Content	The course content must be designed to be presented in an organised, clear, and concise manner, and it must be relevant to fulfil the learning objectives.
Teaching Methods	The teaching methods must be varied to respond to the diverse needs of the students. This can include interactive activities, discussion questions, and educational videos.
Monitoring and evaluation	It is vitally important to measure students' progress and provide information on their performance; for this, the teacher must give constructive feedback to students to improve their learning.
Collaboration and social interaction	In e-learning, the environment is essential for the correct development of learning. In this sense, it is relevant to incorporate instances of cooperation, such as discussion forums and internal messaging.
Effective organisation of time	The planning of the activities must consider the time necessary for the students to carry them out, it must also be clarity in the course calendar as well as in the relevant dates so that students can organise their study time effectively.

The decisions involved in ID are detailed below, based on the principles mentioned above.

3.1.1. Learning Environment

3.1.1.1. Nature and Characterisation of the ECC Course

The focus of the course integrates computational chemistry, pedagogy, and chemical knowledge, supporting the use of scientific databases and Research-Grade Computational Chemistry Software (RGCCS) for the three-dimensional and transformational understanding of chemistry applied to a scientific investigation. In this aspect, the development of the course contributes towards a canonical PSK. In addition, since it is a course aimed at in-service chemistry, biology, natural sciences, or related areas teachers, it accounts for users with a personal PSK.

The instructional needs reported after the pandemic indicate that in-service teachers need to strengthen the TK, TPK', and TSK constructs [70]. Responding to the reported needs is possible based on the general elements an ID should include to build an e-learning course (Figure 1). For this, it is suggested as a pedagogical strategy to incorporate e-PBL aspects in the development of ID, mainly those linked to using problem scenarios based on SSI, according to the guidelines set forth by ESD [71].

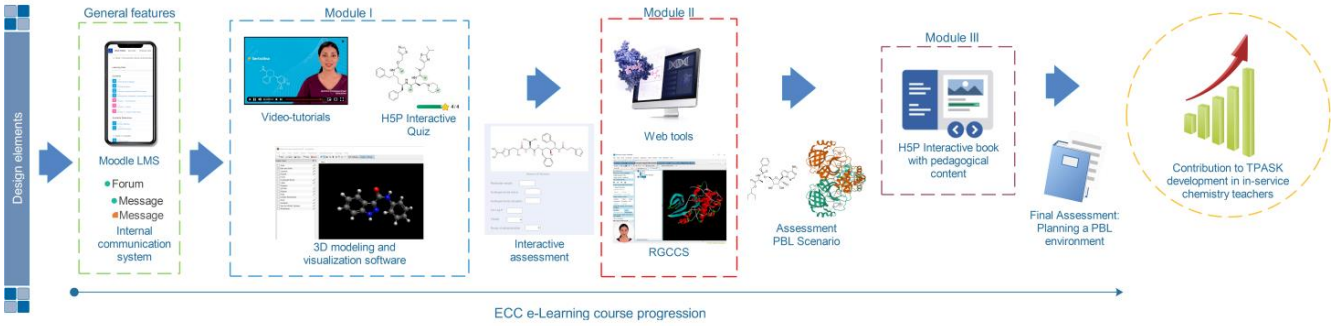


Figure 1. Scheme of ECC e-learning course progression.

Likewise, previous studies of our group highlight the need to incorporate RGCCS as part of the ECC [9,10] because they allow the development of skills such as the interpretation of computational models or the use of scientific protocols, which are necessary to develop TSK. From the ECC, 3D visualisation is fundamental since, for understanding chemical concepts, the teaching activities for learning must be structured around the levels of interpretation of chemical knowledge (macroscopic, submicroscopic, and representational). In this sense, 3D visualisation is an adequate tool since it promotes the understanding and construction of abstract concepts [72–74]. In the same way, molecular modelling is positioned as a fundamental computational chemistry tool since 3D visualisation allows rational interpretation, for example, of the interaction process between a protein and its ligand. It also provides vital information that predicts the system's behaviour. The main reports indicate that this tool generates better learning environments and promotes understanding of concepts [75,76].

Additionally, Fernandes, Rodrigues, and Ferreira [56], based on a systematic review of the literature, report that in-service science teachers show little progress in using innovative technologies, multimedia environments, and websites. Additionally, they indicate the need to incorporate these tools as instruction linked to ID to contribute to TPK.

Architecture and Support during Implementation

This study determined to use the Moodle platform version 4.1 as LMS because it is a free and open-source, it also offers a set of tools focused on students and the learning environment, a simple interface, continuous improvements in both design and security, it is customisable and has more than 43 million courses and 350 million users [77]. Additionally, this open access platform allows teachers in training to acquire the experience of navigating and using Moodle, which directly contributes to their TPK'.

The content organisation was carried out sequentially (Figure 1), where in the course, participants must progress in each activity to move towards the next section. In this sense, navigation through the course is not free but is delimited by sections and their corresponding evaluations, which allow passage to the next section, allowing to organise the content following what was proposed by Chen [78], who, based on a systematic analysis of the literature, realises that a poorly organised self-instruction e-learning course confuses students who could drop out.

Regarding the course modules, its progression shows in the first instance that the teacher, the participating teacher takes on the role of a student in the e-PBL context, aiming to develop their TSK through elements of computational chemistry. Secondly, through activities related to the development of PSK, the participating teacher reflects upon and becomes aware of the learning acquired in the previous module, along with the pedagogical aspects involved (PSK). All of this is done for the teacher to achieve, in the third stage, the connection between TSK and PSK, ultimately projecting this knowledge into their teaching practice and thereby demonstrating their TPASK.

Generation of Content and Interactive Material

In general, the LMS is developed using a programming language specially adapted to web development. For this reason, the courses present preloaded tools that allow content generation. These tools will enable the incorporation of text, images, sound, video, and hyperlinks. Similarly, the evidence shows the use of external tools that allow the incorporation of online resources, such as Google Docs [79] and Padlet [80].

Concerning the generation of audiovisual content, Lu and Kwan [81], from a perception study with chemistry teachers, report that video instruction favours the acquisition of concepts and skills. Along the same line, Jordan et al. [82] report that video instruction, using short videos, facilitates the acquisition of instrumental techniques when it does it before the realisation of practical laboratory activities.

Physics Education Technology (PhET) simulators have also been reported, which can be incorporated directly into the course environment since they are open access and can be run online. Mellizo et al. [83], in a study on the effectiveness of the autonomous use of simulators linked to chemical phenomena, report that simulators allow the generation of significant learning. Along the same lines, Ben Ouahi et al. [84] report the findings obtained from a survey of 114 science teachers on using simulators in instruction, showing that simulators improve learning activities and understanding of scientific concepts.

3.1.2. Technological Tools to Support the ID Process

Generation and Development of Materials and Interactive Content

Following what was explained in Section 3.1.1.3 related to using videos as instruction, this study used a video generation system through Artificial Intelligence (AI) mediated by the Synthesia platform (Synthesia, London, United Kingdom), which uses avatars with photorealistic appearance and movements who position themselves as virtual teachers. Videos´generation is done from the program platform employing a text script, in this case in Spanish, which is interpreted by the AI and adjusted to a selected avatar. Later, through an editing process, it is possible to adjust the speed of the text and incorporate design elements into the video (Figure S4). This way, technical disadvantages linked to sound quality, video formats, and production are avoided. Due to the above, AI software is positioned as a powerful and versatile tool, like a complement to create attractive, high-quality audiovisual content in various languages, with a learning curve that increases rapidly at the beginning and needs low editing times. The generated videos are hosted on the YouTube platform for easy handling and access (https://youtube.com/playlist?list=PLozAiXUC8e7VOTwU7JoSepbUPqBnOTA_R (accessed on 21 June 2023)) (Figure S5).

Similarly, the creation of interactive content was carried out using the HTML5 package (H5P), which allows the collaborative generation of free and open access content through JavaScript. H5P is a free tool for creating interactive content quickly, easily, and with high compatibility with various LMSs. H5P is a native Moodle complement through which dynamic assessments, quizzes, and interactive books were generated. The use of H5P has increased in recent years, and several studies show that it enriches the educational scenario by incorporating interactive content [79]. In addition, H5P has a wide range of templates that will enable any teacher to customise, edit, and create quality interactive contents to suit their specific needs, which can be used in multiple virtual learning environments.

Computational Chemistry Elements

The utilisation of computational chemistry elements such as molecular modelling and 3D visualisation has been widely reported as promoters of the construction and understanding of abstract models that enhance scientific learning [85–90]. Based on the classification of computational chemistry resources that can be used in educational contexts, proposed by [10] and to facilitate its installation, use, and distribution, free and open-source resources were selected as well as multiplatforms, such as:

- Autodock

Autodock4 (version v4.2.6, Scripps Research Institute, La Jolla, CA, USA) is a program that brings together a set of molecular docking simulation tools. This process involves the prediction of ligand conformation and orientation within a specific binding site, involving algorithms and scoring functions that allow predicting biological activity by evaluating interactions between compounds and potential targets [91]. Both Autodock4 and its graphical interface, AutoDockTools, are available as free and open source software for Microsoft Windows, Mac OS, and Linux systems,

Although there is ample evidence of the use of Autodock4 in the search for and development of potential drugs against Cancer, HIV, and COVID-19, among other diseases [92–97], its use has also been reported in the training of students in areas related to medicine, bioinformatics, and education [10,98–100].

- Avogadro

Avogadro (version v1.2.0, © 2022 Avogadro Chemistry) is a free, open-source molecular visualisation, creation, and analysis program. It is available for Microsoft Windows, Mac OS, and Linux systems. It has an extensive library that allows you to use different file formats and a battery of complements that facilitates the incorporation of functions linked to other fields, such as the design of drugs, materials, and simulations, among others [74]. As with Autodock4, a significant amount of the literature reports using Avogadro in specific scientific aspects [101–103] and developing various development activities teaching linked to chemistry [104–106].

- Discovery Studio

Biovia Discovery Studio (Biovia Discovery Studio, Dassault Systèmes Corporate, Massachusetts, USA) is a software package that allows for pharmacophore analysis, molecular dynamics, and protein structure analysis, among other functions [107–109]. In addition, it has a high-quality graphical interface, which allows interactive 3D visualisations. Due to these features, it is only available for 64-bit systems with Microsoft Windows or Linux.

- Virtual Compound Libraries

Molecular synthesis has been a field of scientific work for over a century. However, few infinitely many compound variants have been prepared and studied. With technological advances, the ability to build complex molecules has increased considerably and continues to grow as new reactions are discovered, known ones are improved, and the mechanisms involved are better understood. Based on the knowledge accumulated about the synthesis and analysis of chemical compounds, there are currently databases that collect not only the compounds but also a large number of physicochemical and pharmacological properties of organic and inorganic compounds [110]. Some of the most widely used open access databases are:

a. Drugbank (https://go.drugbank.com/, (accessed on 21 June 2023)): a database containing information on drugs, drug targets, approved biological products, and protein sequences;
b. PubChem (https://pubchem.ncbi.nlm.nih.gov/, (accessed on 21 June 2023)): It is a chemical database. It mainly contains small molecules, nucleotides, carbohydrates, lipids, peptides, and chemically modified macromolecules. It also collects information on chemical structures, identifiers, chemical and physical properties, biological activities, patents, health, safety, and toxicity data;
c. ChEMBL (https://www.ebi.ac.uk/chembl/, (accessed on 21 June 2023)): is a database of bioactive molecules with drug-like properties. It combines chemical, bioactivity, and genomic data to help translate genomic information into effective new drugs;
d. Protein Data Bank (https://www.rcsb.org/, (accessed on 21 June 2023)): is a database of protein structures containing information on the 3D forms of proteins and nucleic acids, with more than 200 thousand structures generally obtained by X-ray crystallography or magnetic resonance. It is used daily by researchers and students to

understand aspects related to molecular biology, structural biology, computational biology, and biochemistry.

ID Monitoring and Evaluation

The course design incorporated a forum to favour internal communication, in which students and teachers can generate messages to the community to raise doubts, upload images, and make suggestions. This activity is asynchronous since participants do not access the system simultaneously; however, participants can subscribe to the discussion to be notified via email when new messages are added to the forum. A private messaging system has also been incorporated, which allows messages to be sent between course users.

On the one hand, it is possible to monitor the course participants' progress by reviewing their interactions with the different sections of the program. An example would be to analyse the activity of the students in each module, as shown in Supplementary Figure S6, where the interaction of five students with the evaluation "Draw structures using the Avogadro software" is evidence. It is observed that three students do not present interactions after a certain period. In this case, contacting them directly through the course's internal messaging is possible. On the other hand, the registration system of all course events can be analysed to characterise the specific interactions of each participant. Supplementary Figure S7 illustrates this internal course logging system, which collects information about the time, user, context, system component, event, description, and path to the system.

Regarding course objectives evaluation, they are assessed at the end of each module, where prerequisites have been established for the activation of the next module, which the participant must complete. For example, module 1 comprises three assessments: (i) drawing a structure with Avogadro software, (ii) identifying hydrogen acceptors/donors, and (iii) evaluating parameters using Lipinski's rule (Figure S1). Only when the participant has completed all the evaluations will the following module be activated. Supplementary Figure S6 shows the event log of a participant who has completed the first task of module 1. In this case, the system sends an alert to the course instructor, who reviews, grades, and provides feedback on the submission. The scores earned in each module contribute to the participant's final mark in the course. This mark was calculated using 40% of the marks from modules I and II and 60% from module III are employed. These percentages are based on the complexity and time required to complete the activities in each module.

Once the course has been completed, evaluating the design and implementation decisions is essential. Hence, course participants participated in several feedback instances, including perception surveys and a focus group, to gather information on the impact of the course on their learning and future teaching tasks, as well as relevant information that allows updating or improving the implementation of the course. This information made it possible to reorganise content, evaluate the usability of the interactive material, and measure application times and ways of using the Moodle system. Therefore, the following versions of this course will be more beneficial since it considers the needs presented by the students during their instruction.

3.1.3. ECC Course Description

The ECC course presents eight sections, within which the first two give the general organisation of the course and presentation of objectives. Also, in this section, participating teachers must sign a consent document that informs them that all information collected during the course will be used for research purposes. This information will be used in a way that does not allow the identification of any individual. Additionally, at the end of the course, participants in the focus group must sign another informed consent document to confirm their participation. These documents were evaluated and approved by an accredited ethics committee in Chile.

The following sections are organised according to three learning modules, being these:

1. Introduction to Computational Chemistry for Science Education;
2. Virtual screening, visualisers, and molecular editors in pedagogical contexts;

3. Fundamentals of PBL.

Modules 1 and 2 are positioned towards the contextualisation of molecular modelling and use of computational tools based on two problem scenarios: (i) evaluation of 3D structures of compounds with pharmacological potential, and (ii) determination of potential inhibitors of COVID-19 linked proteins as socio-scientific problems, both modules contribute to the development of TSK (Figures S1 and S2).

Module 3 provides the fundamentals of PBL and reviews PBL experiences related to chemistry in university contexts. This section is positioned from PSK by showing the methodology and pedagogical strategies that incorporate the method of PBL in chemistry (Figure S3).

Each module additionally presents partial evaluations that contribute to a comprehensive assessment at the end of each module. This evaluation includes the design of learning environments using computational chemistry and creating multimedia content to integrate technology in science education, seeking to contribute to the development of TPASK by teachers.

3.2. Perception of the Participants of the ECC E-Learning Course (RQ2)

The discursive episodes collected from the focus group were carefully categorised based on previously outlined characteristics and research questions formulated in the context of this study. Some of the extracted text passages are presented below for illustrative purposes, which offer the participants a valuable perspective regarding the issues addressed in the study.

(i) Experience with the virtual environment of the ECC e-learning course.

The findings show a positive perception of the virtual environment and the course's organisation.

On the one hand, the course structure shows an organisation that allowed the correct teaching process development. *"The modality of the course was generally very user-friendly, the platform was easy to use (...) it was quite easy to access, and everything was super structured". (Id_3). "(...) The structure and platform used by the course were good (...) it allows you to follow step by step and not get lost along the way, there were also activities that were well organised (...) that is, the structure from the point of view of the educational part was very well structured". (Id_1).*

On the other hand, the use of tools incorporated in the virtual environment, such as H5P, is also highlighted. *"(...) There was an activity that I really liked, it was based on an image together with a brief instruction (...) I imagine that it was not very complex to assemble and that it was based on the functionalities of the Moodle platform" (Id_4).* And the use of the system messaging platforms. *"(...) The very quick answers from the person behind the course also helped me (...) because you ask a question and after 30 min or 1 h, he would answer and solve the problem (...) that helps, because I was working at home trying to make the process resolve the activities and since they responded quickly, I could continue the process quickly as well". (Id_1). "I think he was texting every day because he was like can you help me with this? (...) and they always responded". (Id_3).*

(ii) Facilitators for learning chemistry and science in general.

There is evidence of a positive assessment towards using videos to teach the modules. *"(...) what I liked the most in each module was the part with the videos (...) they kept you connected with the topics, they clarified the ideas and allowed you to illustrate what had to be done graphically (...) in the last part of the processes, where you had to do the calculations, although there was the page with the text and graphs, the video was more useful to me". (Id_1). "(...) It was easier for me to listen to the video in the background while I was practising step by step with the program, so it was very successful. It made it much easier for me to progress". (Id_6). "(...) I loved the use of artificial intelligence in the videos because it brings not only us but also the students closer to an artificial intelligence where interpretation is sought in the videos, which was also very in vogue (...) a little while ago, I don't know if today or yesterday I reminded myself that there was a presenter in the*

United States based on artificial intelligence, so each time it is going to be inserted more into our society and what better way to do it through education". (Id_3).

(iii) Computational chemistry or Cheminformatics: uses, knowledge, and skills.

Regarding computational chemistry tools, they mainly focus on using open access tools, such as scientific databases and visualisation software. *"(...) all the software was open access (...) anyone could access the specific scientific information, totally free, they did not require registration or anything (...) it was downloaded from the official page and used immediately (...) even, the issue of databases could be done directly by accessing the Internet (...) it can even be done with a mobile phone". (Id_4). "(...) I think that the most useful thing was the visualisation using Avogadro (...) I had already used it a long time ago, but I couldn't remember". (Id_2). "(...) I think that where I learned the most was in the docking section, using Autodock (...) now, I have the confidence to use Autodock and follow the entire flow of the docking process". (Id_1).*

Regarding acquiring knowledge, they mainly focus on the general theme of the course related to pharmacological issues. *"(...) I found it quite relevant to investigate the different drugs and their components in more depth and to bring that information to a piece of data. It greatly impacted my learning". (Id_6). "(...) For me, the Lipinski rule was exciting (...) one knows that drugs go through certain stages before being administered orally or in another way, but I had no idea about this rule (...) for me, it was a novelty". (Id_3). "(...) The relationship of everything with pharmacology (...) made the relationship of chemistry with biology, medicine and other areas closer (...) I learned a lot in the relationship of computational tools —computational chemistry tools— in an interdisciplinary way." (Id_4).*

Concerning the acquisition or development of computational or computational chemistry skills, a positive evaluation is perceived towards elements linked to scientific information, simulation, and 3D modelling. *"(...) search for data in a specialised chemistry database. Searching for a particular data of a compound and obtaining its properties no longer has any complexity. It is the minimum complexity of using a browser or a web page (...). When one uses scientific software, you can develop many skills that sometimes go beyond the specific contents of chemistry or biology, and it has to do with the use of technologies, which can be enriching". (Id_4). "(...) I learned a little more about computational chemistry, more than the chemistry itself, because chemistry like that in general, I think I handle it, but I did learn a lot about computational chemistry, software, and the use of databases." (Id_5). "(...) in my case, I felt a greater development in the analysis and evaluation of information (...) in all the so-called higher-level skills (...) because I feel that the difficulty level of the module was quite high." (Id_2). "(...) I believe that the essential skills that I can take away from the course are the use of models, the use of digitisation itself (...) is to put a new learning modality in front of a computer and front of the student, that it is not only in the notebook, in the book or even in the laboratory (...) now with digitisation everything is easier." (Id_3).*

(iv) Generation of a PBL environment and projections in their teaching work.

On the one hand, there is evidence of a positive assessment of the stages of the course that allow the development of a learning environment. *"(...) the course and the use of technological tools favour us and enrich our cultural baggage, so to speak, to take classes (...) we go through everything, use simulators, search for information and then solve a current problem (...) the different stages of the course allowed us to develop different things, acquire knowledge about databases and other particulars of chemistry, as teachers we developed pedagogical knowledge because, after all, we were thinking about how to modify this to apply it to the school or implement it in the future". (Id_2). "(...) I was struck by the idea of 3D visualisation (...) to bring to the concrete something very abstract and that in school students are told, "imagine a key and a lock", but now I could say, look at this clearer example and then use the software". (Id_3).*

On the other hand, the time required to implement a PBL environment is revealed as the main obstacle. *"(...) it is relevant to have the time available to generate all the materials such as the video tutorial to use the software, the didactic material to be used or the evaluation instruments (...) so I feel that these are like the difficulties that could have". (Id_2). "(...) as difficulties, I think it is time to design a module (...) the fact that one has to do all these activities from scratch and plan them, it could be a bit exhausting (...) there is a lot of work behind the implementation of a*

PBL environment". (Id_4). "(...) time is the great limit that we have at a general level, the time for planning and putting activities into practice". (Id_3).

The assessment is positive regarding the projection of what was done in the course. *"(...) I had few technological tools to be able to apply them in a school context (...) now I can connect the technologies with the class in a more coherent line of deepening". (Id_6). "(...) for me, the course is a sum of tools that I am going to use (...) I already have some elements in my class planning". (Id_3).*

4. Discussion

4.1. ID for ECC E-Learning Course and Technological Support

There is little evidence of using ID models for chemistry courses and even less for e-learning chemistry courses. However, the authors realise the importance of identifying topics, forms of instruction, organisation of contents, and creation of materials. These do not directly adhere to a particular ID model, but it is possible to characterise them as stages within a rather generic model.

It is possible to distinguish that what is reported in the literature regarding ID linked to chemistry courses can be linked to some design stages. A clear example is reported by Busstra et al. [111], who developed an e-learning course on chemical analysis in food and indicated as fundamental stages of the design the creation of resources, evaluations, and their implementation, which is consistent with what is proposed by the ADDIE and ICCEE (an acronym for Identification, Choosing, Creating, Engagement, Evaluation) models [15,69]. Similarly, Al Mamun et al. [112], in the framework of an e-learning course on thermodynamics, suggest an ID based on strategies and skills needed by students to analyse a scientific problem. In this sense, this design would agree with that proposed by Jonassen's [12] model.

However, two fundamental phases must be included in any e-learning ID process:

The first relevant stage is engagement. This stage accounts for the need to incorporate actions in the ID that guarantee a motivating and attractive learning environment that commits course participants not to drop out. This line is based on three activities: (i) feedback on progress, which allows students to demonstrate their progress; (ii) interaction with other course participants; it is essential to link students with other participants through messaging, discussion forums, and debate; and (iii) direct connection, participants become involved in the subject matter of the course when they actively learn, taking roles and decisions about their practice [113].

The second relevant stage involves the positioning and flexibility of the ID model, which is based on the student, in this case, in-service chemistry teachers. In this line, internal communication is a crucial aspect of monitoring the progress of the course during its implementation. This communication involves interaction between teachers and course participants, underlining the importance of integrating communication and collaboration tools into e-learning systems.

This ID also incorporates the selection of technological resources that allow the development of the course. In this sense, Moodle has an advantage due to its features and the community that supports it. The ability to embed almost any type of content allows for a dynamic ID following current emerging technologies. In addition, the Moodle system provides the collection of whole interactions made by its users during the completion of the ECC course. It includes event logs, learning results, and learner profiles. These records can be transformed into relevant information through data mining techniques, allowing to obtain significant information that allows making decisions about ID to improve student learning processes (Figure S7).

4.2. Development of TPASK through the ID of the ECC E-Learning Course

Concerning the design decisions that contribute to the development of TPASK constructs, the course modules' sequencing was crucial—developing three instances linked to specific constructs made it possible to deploy formative situations more effectively.

Along these lines, computational chemistry tools serve as excellent support for developing TSK based on problem scenarios (Modules 1 and 2). Similarly, the methodology used provided relevant pedagogical support for teachers to practically demonstrate the pedagogical considerations following the course, thereby contributing to the development of PSK (Module 3). These contributions to the knowledge bodies mentioned above allow the emergence of TPASK in teachers who, through developing a solid connection between TSK and PSK, have generated teaching proposals rich in technological and scientific knowledge, clearly showcasing significant progress in their personal knowledge development.

Based on the TPASK model, our group gives an account of the Technological Pedagogical Chemistry Knowledge (TPAChK) model, from where the concept of ECC emerges. The ECC is a new construct that seeks to distinguish the knowledge that a teacher who designs, develops, and implements learning sequences that integrate computational chemistry tools to support the development of chemical knowledge in their students. One of the fundamental elements of this type of knowledge—TPAChK—is the teacher's ability to implement practical activities with computational chemistry tools. This skill implies that they must be able to identify the type of software, database, hardware requirement, practical exercise, problem, or authentic problem that is more relevant to the level of development their students have. Additionally, they have to be able to implement student-centred hands-on learning methodology (e.g., problem/project-based learning) and appropriate assessment methods.

The authentic problems and even practical exercises teachers can address for the design of learning sequences require knowledge related to some of the main aspects that allow problem-solving from the perspective of computational chemistry as a constituent element of Technological Chemistry Knowledge (TChK). In good agreement with Tuvi-Arad [114], we can summarise these TChK aspects in (i) selection of a computational method or technique, (ii) optimisation or calculation of molecular or supramolecular structure, (iii) calculation or obtaining of molecular, supramolecular or physicochemical descriptors, (iv) generation of a chemical model or simulation, (iv) analysis of the generated model, and (vi) scientific visualisation of the model or simulation. The teacher's ability to make decisions regarding the selection, sequencing, and iteration necessary to address an authentic problem in a pedagogical setting will be vital in implementing a successful learning module. Additionally, this decision-making brings into play the teacher's TSK' that accounts for the non-linearity in the knowledge generation process in the science field, and also the level of approximation implicit in the selected calculation methodologies, the validity of the results obtained and limitations of the scientific models present in the design.

The discursive episodes about the perception of in-service teachers who participated in the ECC e-learning course show that using RGCCS is an effective way to enhance scientific skills, such as data processing and analysis of scientific evidence. These skills allow the development of scientific research and the generation of PBL environments that integrate digital technologies based on scenarios that involve real problems.

In this line, teachers have more easily acquired knowledge in the area since, during the pandemic, they were forced to strengthen their technological skills (TK). This technological competence becomes the basis for effectively developing other bodies of knowledge, such as TSK and TPK'. In this way, teachers are better prepared to explore innovative teaching strategies, promote interactive learning experiences, and adapt to the changing educational landscape.

The development of TSK is evidenced in the same way in the participants' perception related to the incorporation of computational chemistry tools in their learning process. In this line, teachers demonstrate the appropriation of the use of scientific databases, as well as modelling software. Furthermore, the participants realise that using RGCCS allows modelling and visualising in 3D components that are often abstract, such as protein–ligand interaction, favouring the understanding of scientific knowledge for designing learning activities, contributing directly to the construct TPASK. However, the use of non-teaching time emerges as a great obstacle to this process since teachers, although they have the

necessary knowledge to create a learning environment using technologies (TPK′), reveal that the time to prepare for these teaching experiences learning is insufficient.

Based on the above, the ID, together with the development of TPASK, allows for innovation in the generation of e-learning courses contributing to the development of challenging learning activities from computational chemistry tools [90].

5. Conclusions

This research identifies some fundamental elements necessary for an e-learning instructional design integrating the ECC and e-PBL from the literature overview. Among these essential elements, the following stand out: the use of an intuitive and easy-to-use learning management system (i.e., Moodle), the definition of clear learning outcomings using a modular way, the effective sequencing of the knowledge bodies (i.e., $TSK \rightarrow PSK \rightarrow TPASK$), the selection of a methodology student-centred and with a focus in authentic problems, the implementation of monitoring and continuous evaluation, the provision of constructive feedback, and the guarantee of efficient time management. This design allowed the development of the ECC e-learning course, supported by resources from cutting-edge technological tools, such as RGCCS, artificial intelligence, and H5P.

The perception of the teachers regarding the course was positive, evidencing an incipient development in terms of the potential integration of technological tools and RGCCS, as well as an interest in the use of PBL as a methodology to improve the quality of teaching and understanding of scientific concepts by students.

In practice, the realisation of this course contributes as a vehicle that allows the development and complementing of the bodies of knowledge linked to the TPASK of in-service teachers. Although teachers show better preparation and greater use of new technological tools compared to pre-pandemic reports, the use of these tools does not necessarily guarantee a deep understanding of the potential of technology in teaching and learning. Therefore, teachers must acquire technical skills and a critical knowledge of the use of technology in the classroom and its impact on student learning.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/educsci13070648/s1, Figure S1: Mock-up ECC Course—Module I: Introduction to Computational Chemistry for science teaching, mounted on the Moodle 4.1 system. Figure S2: Mock-up ECC Course—Module II: Virtual screening, molecular viewers and editors in pedagogical contexts mounted on the Moodle 4.1 system. Figure S3: Mock-up ECC Course—Module III: Fundamentals of Problem-Based Learning, mounted on the Moodle 4.1 system. Figure S4: Synthesia STUDIO Dashboard. Figure S5: Youtube ECC e-Learning course playlist. Figure S6: Control panel to monitor participation in the ECC e-learning course. Figure S7: Tracking log of all ECC e-Learning course events. Table S1: Computational chemistry resources in educational contexts of computational chemistry. Table S2: Focus group script. Table S3: Main ID models reported in the literature.

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