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A framework for the development of Pedagogical Process Simulators (P2Si) using explanatory models and gamification

Simoneta Caño de las Heras, Carina L. Gargalo, Charlotte Lærke Weitze, Seyed Soheil Mansouri, Krist V. Gernaey, Ulrich Krühne

1. Introduction

Industrial chemical and biochemical engineering, as well as the training and education of engineers, is under continuous evolution. These fields are going through exciting times in adapting sustainable practices and taking an active part in the transformation towards digitalization paving the way to Industry 4.0. Industry 4.0 (or smart manufacturing) is the ongoing transformation of traditional manufacturing using modern smart technologies. Therefore, digitalization and automation are key players to achieve smart manufacturing. At the same time, this can result in more sustainable processes by, for example, increasing process efficiency (Narayanan et al., 2020; Clomburg et al., 2017; Gargalo et al., 2020). Meanwhile, higher education, including in the field of process systems engineering, is facing challenges such as: (i) the accommodation of an increasing number of students; (ii) the need to teach practical aspects of complicated processes; (iii) the need for a more flexible educational system; and, (iv) the students’ preparation to actively take part in the transition to Industry 4.0. The first two points have been widely mentioned among the needs and challenges of engineering education (Baroutian and Kensington-Miller, 2016; Hofstein and Lunetta, 2004; Koretsky et al., 2011; Feisel and Rosa, 2005). On the other hand, flexible learning reflects the current need of adapting to evolving requirements, time and location of study, as well as teaching methods, assessment, and certification (ANTA, 2003). This is especially important due to recent events, such as the Covid-19 pandemic, where, according to UNESCO (The United Nations Educational and Organization, 2020), by...
March 3rd 2020, 87.6% of students worldwide were out of their educational institutions. Therefore, a new paradigm in education arose, in which the demand for more tailored online platforms, even if this was not new, has become urgent (Jeffery and Bauer, 2020; Dietrich et al., 2020). In addition, the development of such platforms supports the UN Sustainable Development Goals, in particular Goal 4 - Quality Education. By 2030, the UN aims to "ensure equal access for all women and men to affordable and quality technical, vocational and tertiary education" (United Nation Development Program, 2014). Digital platforms could facilitate and standardize knowledge sharing and training.

Moreover, in the age of digitalization and the transition to smart manufacturing, process models have gained even more relevance. Process models can be an unambiguous way of reporting and exchanging knowledge as they combine mathematical expressions with process information (Narayanan et al., 2020). Therefore, when the aim is to teach a certain process, the educational system and its methods should adapt in order to echo the new trends and challenges faced by the industry today. To achieve this, the curriculum should be updated so that topics involved in the digitalization of the industry, such as model generation, validation, maintenance, and model-based decision-making, have a greater weight (Cameron et al., 2019; Kiss and Grievink, 2020). In this way, future engineers will be better prepared to face the challenges and embrace the opportunities brought by ongoing developments in the industry.

Hence, there is a clear demand for flexible and adaptable educational digital platforms that tackle the current challenges and embrace opportunities created by the unfolding developments in the chemical and biochemical industry. Nevertheless, those digital platforms should not forget their educational aim and must be able to motivate and attract the students.

In chemical and biochemical engineering classrooms, computer-aided tools have been the most common digital platforms used to teach processes. These tools, also referred here as simulators, can reproduce phenomena (e.g., kinetic reactions, filtration, etc.) under different conditions and, when used in education, they can help the students to gain theoretical knowledge and conceptual understanding (Feisel and Rosa, 2005; Balamuralithara and Woods, 2009). Moreover, simulators are able to engage students in intuitive learning, based on action and the possibility to control and explore the embedded process (Shen et al., 1999). On these grounds, simulators have been used as learning tools since the 1970s in many fields within science and engineering (Forbus et al., 1999; Tjärnberg et al., 2017; Kerala, 2007; FunctionBay, 2007; Ferrero et al., 2002; Guimarães et al., 2003). Specific examples of simulators commonly used as part of bachelor and master curriculums of chemical and biochemical engineering are: PROII (Software, 2015), Aspen Plus, Hysys (AspertiTech, 2017) and SuperPro (Inc., 2017). These simulators have been designed to allow for rigorous design and analysis at the early stage of the process' conceptual development. As a result, they can accurately represent complex process systems, which brings great benefits to the students. However, these tools require a high level of process understanding, and thus it is difficult to use them to teach fundamental concepts. They lack an integrated learning design as well as motivational elements. In recent years, specific simulators have been created as learning tools for undergraduate engineering and science students such as BerryMaker BACH-BERRY (2017), Labster ApS. (2018), Genomics Digital Lab Spongelab Interactive (2018), Chemlab Modelsience (2019), and CHEMOTION Al-Khalifa (2017). These software tools mainly target theoretical knowledge, and aim to engage the students in learning by using different techniques such as gamification, virtual/extended reality, or hand and finger motion systems. These simulators have been generally used as a replacement or as a complementary tool to the laboratory experiments (Dyrberg et al., 2017; Makransky et al., 2016; Bonde et al., 2014). They are regularly characterized by closed "point-click-observe" type of activities (Caño de las Heras et al., 2021). This type of "point-click-observe" flow is linked to a combination of teaching the academic content (or theory) followed by an assessment of the learning (Abdulwahed and Nagy, 2009). Hence, the use of these tools coupled with laboratory experience, can be beneficial for the students to acquire the intended theoretical and practical knowledge. However, these simulators are not adequate when students aspire not only to understand and apply their knowledge, but also to evaluate and create such information through active experimentation (Abdulwahed and Nagy, 2009).

Besides, while using both types of simulators in the classroom (educational-focused, such as LABSTER, or for rigorous design, such as ASPEN HYSYS), students have found several areas for potential improvements, such as the lack of collaborative and customized learning (Dyrberg et al., 2017; Caño de las Heras et al., 2021). Moreover, the students have also pointed out that process models are neither introduced nor adequately explained in either type of simulators. This is in clear conflict with the urgency to educate and prepare students for a digitalized industry.

Therefore, the next generation of simulators should combine the best features of each type of simulator while tackling the identified areas of improvement, as well as being flexible, rewarding, adaptable, and scalable to the users' future needs (Fig. 1).

To achieve this, some questions must be answered: (i) How can digital platforms facilitate the teaching of processes? and (ii) what should the design considerations be for such process simulators? An educational simulator must have a learning design. A learning design is composed by the learning goals, the settings in which learning will take place, the content, the learning theory and methods used, the conditions of the evaluations, and the prerequisites of learning (such as previous knowledge) (Hiim and Hippe, 1997). If the simulator lacks a proper learning design, the student might feel disengaged, and the pedagogical value of the simulators will decrease. To be able to keep the student engaged.

![Fig. 1. Schematic representation of the needs for the next generation of pedagogical simulators.](image-url)
during a continued period, the simulator should provide open exploration while, ultimately, allowing for the creation of its content. In this way, the learning goals of a successful simulator should follow the Bloom’s Taxonomy, in which a new topic is (i) memorized, (ii) understood, (iii) applied, (iv) analyzed, (v) evaluated, and (vi) created (Krathwohl, 2002) to achieve the metacognitive domain. In addition, the level of motivation is another important contributing factor for student engagement. The affecting aspects that arise from actively learning and participating have inspired the development of different strategies to boost students’ motivation. Gamification is one of these strategies, where game elements are applied in non-game contexts (Deterding, 2012). Although it has been successfully implemented in several areas (e.g., business, marketing, corporate management, etc.), the implementation of gamification in engineering education is still not yet well established (Dicheva et al., 2015; 2018). Several examples of educational software tools that integrate gamification used in civil engineering (Ebner and Holzinger, 2007) or computer science (Jayasinghe and Dharmaratne, 2013), have shown an increase in incidental learning and student engagement. However, a reproducible pathway for the integration of game elements into a process simulator is still missing.

Moreover, there is a need to develop a user-friendly approach to introduce and teach process models to the today's students. Process models describe the phenomena that control a system’s behaviour, and therefore, they have a sometimes unexploited educational value for engineering students. Furthermore, as previously mentioned, the transition to Industry 4.0 requires engineering graduates and trainees with knowledge and skill in the creation, validation, maintenance of process models, and model-based decision-making. Lastly, an educational simulator could benefit from not only be designed for students but also by the students. In this way, the functionality and usability tests would be performed as an iterative process during all simulator design stages. Through this collaboration with students as future users, a better human-computer interaction is ensured by providing the platform with more effective communication. Among other benefits, this approach achieves an easier and less confusing user instructions (Gong, 2009).

All these factors should be considered in the conceptual design of a process simulator. However, to the best of our knowledge, no other studies have integrated these principles in a reproducible way for the design and first-stage implementation of a process simulator. Therefore, this study proposes a framework for the systematic development and conceptual design of educational process simulators (P2Si). P2Si aims to establish a holistic process that includes:

i. a learning perspective through educational design;
ii. a motivational strategy by using gamification;
iii. the use and implementation of process models as an educational resource;
iv. the design of the software as a tool for open exploration;
v. the inclusion of the future users (the students) as pro-active agents in the process simulator’s development and design by applying functionality and usability user experiences as well as engaging them in the evaluation of their learning satisfaction.

We believe that the application of this framework will lead to the design of novel process simulators whose sole purpose is to educate future engineers and prepare them for a digitalized industry.

The remainder of this article is organized as follows. In Section 2, the framework is presented and described in detail in a step-wise manner, along with the methods and information required. Section 3 explores the application of P2Si to showcase its usefulness, leading to the development of a digital platform prototype, as a proof of concept. This digital platform prototype is called BioVirtual Lab (BioVL), and is available at www.biovl.com. Finally, conclusions and future perspectives are presented in Section 4.

2. A systematic computer-aided framework for the design of Pedagogical Process Simulators (P2Si)

The proposed framework, P2Si, targets to create a reproducible strategy to construct process simulators with a pedagogical value. The main goal is to achieve the conceptual design of a promising candidate for the teaching of processes while considering the requirements previously described. P2Si is composed of five hierarchical steps (Fig. 2), where three of the steps are designed for construction and solution, while the last two are for application and validation. Noteworthy is that the proposed framework is generic, and consequently, each step can be applied independently based on the availability of information.

2.1. Step 1: Problem identification

This step defines the learning goal and educational purpose to be achieved through the application of P2Si. The learning goal's definition is then supported by quantitative or/and qualitative data gathered from interviewing the students and instructors, and/or from a literature survey. Afterwards, educators must define the learning requirements for the students. For example, if the goal was for the students to learn about enzymatic reactions, the learning goals could be to develop: (1) knowledge on different types of enzymatic reaction mechanisms; (2) skills in the calculation of the kinetic parameters; and (3) competences in performing laboratory experiments of an enzymatic reaction with the objective of collecting data for estimating its kinetic parameters.

2.2. Step 2A: Pedagogical description

This step aims to establish the learning design of the process simulator. In order to do so, the six elements defined in Table 1 must be specified. Table 1 follows a didactic frame proposed by Hiim and Hippe (1997), further used and expanded by Læke Weitze and Ørngreen (2012).

This strategy is based on a series of “if...then...” rules, derived from: (i) theories, (ii) examples, or (iii) patterns (Berggren et al., 2005). The pedagogical description embedded inside the simulator may be redefined during step 4, where the students are co-participants in the design of the process simulator, or in step 5, during the pedagogical verification (information feedback loop highlighted in Fig. 2).

2.3. Step 2B: Mathematical characterization, implementation, and solution

The mathematical development of a process model requires: (i) an overall understanding of the system and the involved phenomena; (ii) the identification of a set of mathematical equations to describe the system; (iii) parameter estimation (if experimental data is available) or use, if possible, of parameters obtained by previous studies; (iv) the implementation of the model and its solution in a computational tool; and finally, (v) the validation of the model through literature or experimental data.

In this work, the simulator’s educational value is the foremost goal; thus, step 2.B focused on providing a clear and structured mathematical description of the process models. Hence, the mathematical development involves two sub-sequential tasks: (1) model characterization and (2) implementation and solution. Firstly, the model is characterized so the students understand the phenomena behind the process, as well as the structure of the equation(s)
that describes it. By taking such an approach, we expect that students will gain expertise to evaluate and create their own models. Secondly, the process model is implemented and solved inside the computer-aided tool. These two sub-steps are described in detail below.

**Step 2B.1 Model characterization**

The process model is described through a series of hierarchical steps as represented in Fig. 3.

This sub-step greatly relies on the collection of trustworthy and understandable information. Hence, literature, databases, model libraries, expert knowledge, experience, and experimental data are required in order to have a complete picture of the available information. In some cases, this can be a highly time-consuming activity as information tends to be unorganized and with significant gaps.

**Step 2B.2: Model implementation, solution, and validation**

This sub-step is focused on the implementation and solution of the process models. The model implementation is a fundamental aspect of practical modelling aspects, and it supports creative and open learning. It is recommended that the model implementation follows a template-based approach (Fedorova et al., 2014). In the available templates, models are decomposed into three divisible classes (Cameron and Gani, 2011): a) balance equations (such as mass or energy balance), b) constitutive equations (such as a
chemical reaction), and c) connection and conditional equations (to describe the surroundings and system connections). As each class can be treated like a block that can be combined to create a new model; students can explore and learn about the construction of mathematical models (de Las Heras et al., 2019) in a structured way.

This sub-step is also susceptible to redefinition based on feedback information from steps 4 and 5, as the process model equations and implementation will be used as an educational resource for the students.

2.4. Step 3: A motivational strategy – Gamification design

The overall aim of step 3 is to incorporate motivational strategies to engage students in learning. Among other strategies, gamification is one of the possible methods to encourage and support motivation, as well as a strategy that provides an enjoyable experience to the students (Weitze, 2016; Kiill, 2005). Other strategies that can be used for the same purpose are, for example a specialized learning design such as game-based learning, and/or new technologies such as virtual reality (VR), or augmented reality (AR). It is important to highlight that both AR and VR can be used in combination with or even to replace gamification as the motivation strategy used in step 3. In this work, the proposed framework only incorporates gamification based on the benefits related to the easiness of its implementation compared to the previously mentioned new technologies.

Gamification, when used to develop a gamified scenario, has shown positive results in transferring knowledge, competences, and skills that allow students to adapt to new situations (Blumberg and Fisch, 2013; Hodent, 2017). The use of gamification brings the possibility to provide the students with immediate feedback in an engaging scenario, which cannot be obtained in real life. For example, a newly graduated engineer can confront an accident that will change the temperature of the process and immediately see the effect on the fermentation process simulator in contrast with reality, where accidents must not happen and sometimes the effect of such change would only be observed after several hours. In addition, in a gamified scenario, the effect should involve memorable feedback (e.g., a representation of dying microorganisms).

In this work, the Smiley model (Lerke Weitze and Ørningreen, 2012), as presented in Fig. 5, has been proposed to integrate the learning design and gamification. As the learning design has been defined in step 2A, the current step focuses on creating a playful environment inside the process simulator through the use of different game elements (Fig. 4). It is important to highlight that the Smiley model is not the only available framework for gamification, and the number of game elements that belong to gamification is still a controversial topic (Dicheva et al., 2015; Albertarelli et al., 2018).

Moreover, curiosity, competences, and social relationships are driving forces for the success of learning and engagement in gamification. Hence, those elements should be considered at an early stage of the design of the process simulator.

The design of a successful gamification strategy commonly results from an iterative process with the participation of future users (students and/or trainees). This is due to the fact that the main goal is to create a memorable and meaningful experience, with a challenging, clear and engaging design, as well as a consistent rewards system (Hodent, 2017). Hence, P2Si proposes to involve future users as co-designers through a co-participatory experience. This allows for the evaluation of their motivation to use the process simulator, which includes the application of a series of iterative steps of participatory design and pedagogical verification (as presented in Fig. 2).

2.5. Step 4: Participatory design of the process simulator

“Frighten? Why should anyone be frightened by a hat?” (The Little Prince, Antoine de Saint-Exupéry). This quote demonstrates the importance of the alignment between the mental model of the students and the process simulator, and hence the use of participatory design. In the participatory design step, the students become actively involved in the design process, and their preferences are reflected in the design of a technology they use. Hence, misunderstandings, confusions, and false impressions can be minimized, while the students can develop a sense of ownership and empowerment (Pontual Falcão et al., 2018; Y., 2012).

Some of the participatory design methods are, to name a few, workshops, cooperative prototyping, mock-ups, card sorting, and user design (Y., 2012). Unlike the previous steps, step 4 relies on a social design, and therefore, the outcome highly depends on the group of students who participate in this step. A more detailed example of a participatory design strategy is explained and demonstrated in the proof of concept (Section 3.5).

2.6. Step 5: Pedagogical verification

This is the final step of the P2Si framework. It seeks for confirmation of the process simulator’ value as an educational tool. Consequently, P2Si proposes to evaluate the (i) learning, (ii) memory, and (iii) perception that the students have while using the process simulator. These are key pillars of the student’s cognition (Hodent, 2017; Carroll, 1997).

This framework focuses on evaluating the functionality and usability of the process simulator, as well as its pedagogical value from the students’ perspective (Fig. 5). In order to do so, several methods have been previously designed and used to collect data on these aspects such as questionnaires, interviews, external observers, etc.

To evaluate usability and functionality, due to its importance in human-computer interactions, there are several standardized methods, such as the System Usability Scale (SUS) (Tullis and Albert, 2013) or the Questionnaire for User Interface Satisfaction (QUIS) (Chin et al., 1988), among many others. Meanwhile, it is also important to collect combined data through, for example, the introduction of an external viewer inside the pedagogical verification. Through observations, the external viewer will have a more realistic idea of the students’ interaction with the software.

To conclude, based on the sequence of the construction and validation steps, the user of the framework should arrive at a conceptual design of an educational process simulator using explanatory process models and gamification.

3. Proof of concept

To showcase the applicability and usefulness of the proposed framework (P2Si), a proof of concept is developed in the form of a digital platform prototype (BioVL). BioVL is a conceptual design of a bioprocess simulator to meet the demand for a more efficient and higher quality bio-manufacturing education for the students and trainees, as the requirements for flexibility and creativity increase (Noorman and Heijnen, 2017). In this work, we envision BioVL to be included in the chemical and biochemical engineering undergraduate curriculum.

3.1. Step 1: Problem identification

A typical setup in universities’ (bio)laboratories is to teach to undergraduate students the aerobic growth of Saccharomyces cerevisiae on glucose and ethanol (Østergaard et al., 2000). This process usually spiked the students’ interest since it is a process with
Fig. 4. (a) needed elements for the integration of gamification elements into the learning design, based on the Smiley model from Weitze (2016); (b) schematic description of the different game elements in the Smiley model.

![Diagram of learning design and gamification elements](image)

Fig. 5. Schematic representation of the elements that compose the student’s cognition (Hodent, 2017), as well as the evaluation types and methods considered in this framework.

![Diagram of student’s cognition and evaluation methods](image)

applications in many bio-manufacturing industries, such as food, biofuels and pharma productions. However, later restrictions have complicated its teaching in the physical laboratory.

Meanwhile, this system provides the perfect frame to introduce mathematical modelling practices to undergraduate students. The mathematical modelling behind the selected system is well established (Lencastre Fernandes et al., 2012; Sonnleitner and Kappeli, 1986), and as it describes an overflow metabolism, it can also be used for other microorganisms, such as Escherichia coli (Vazquez, 2018). Hence, this system provides the perfect frame to introduce mathematical modelling practices to undergraduate students.

Therefore, this bioprocess has been selected as the show case used in the development of BioVL.

3.2. Step 2A: Pedagogical development

The learning design is defined by following the previously mentioned learning elements (see sub-Section 2.2), and they are detailed in Table 2.

As reported in Table 2, the learning process uses a combination of the Kolb’s experiential cycle and collaborative learning. Kolb’s experiential cycle involves the students in (1) a concrete experience, (2) a reflective observation, (3) an abstract conceptualization, and (4) an active experimentation of their knowledge, and thus, it provides an excellent frame to cultivate logical thinking and problem-solving. The Kolb’s experiential cycle is implemented in the process simulator’s design as a loop of information-action inside the simulator. In addition, collaborative learning allows the students to learn from each other, by sharing and discussing a topic. In the case of e-learning, the other ‘student’ (learner) can be replaced by chats or chatbots (Monahan et al., 2008; Kane, 2016). In this work, a chatbot with artificial intelligence has been designed for the developed process simulator. This aims at improving the human-computer interactions and facilitate learning inside the software. In addition, a novel system built upon two databases has been developed (de Las Heras et al., 2020). These databases are
Table 2
Learning design for the case study.

<table>
<thead>
<tr>
<th>Element</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pre-requisite of learning Setting</td>
<td>Preferable elementary knowledge about fermentation and microorganisms.</td>
</tr>
<tr>
<td>Learning goals</td>
<td>A software/computer-aided tool.</td>
</tr>
<tr>
<td></td>
<td>• To understand the basis of bioprocess and process modelling;</td>
</tr>
<tr>
<td></td>
<td>• To analyse the principles behind the aerobic growth of \textit{S.cerevisiae} on glucose and ethanol, and its mathematical model;</td>
</tr>
<tr>
<td></td>
<td>• To design and implement modifications in the model.</td>
</tr>
<tr>
<td>Content</td>
<td>It covers: (i) the general theory of bioprocesses and modelling, (ii) implementation, and (iii) a more detailed description of the mechanisms behind \textit{S.cerevisiae} growth.</td>
</tr>
<tr>
<td>Learning process</td>
<td>Use of Kolb’s experiential cycle, and a collaborative learning setup between students and a chatbot.</td>
</tr>
<tr>
<td>Assessment</td>
<td>Use of variable feedback and self-evaluation as the students test their hypothesis and develop as well as test abstract conceptualization.</td>
</tr>
</tbody>
</table>

![Fig. 6. Sketch of a \textit{Saccharomyces cerevisiae} cell and the phenomena included in the model. The oxidation of glucose to biomass is presented in green. The reduction of glucose to form biomass and ethanol is depicted in brown. Finally, the oxidation of ethanol to form biomass is shown in blue. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3.3. Step 2B: Mathematical development

The mathematical model of the aerobic growth of \textit{Saccharomyces cerevisiae} on glucose and ethanol has an appropriate level of complexity for undergraduate students. Furthermore, it has well-established kinetic constants and biological parameters (Lencastre-Fernandes et al., 2012; Sonnleitner and Käppeli, 1986).

Step 2B.1: Model characterization

The model explained to the students includes the mass balances and the kinetic reactions. The momentum balance (e.g., the Navier-Stokes equations) is omitted as the understanding of basic concepts is prioritized. However, this translates into the inability of the model to accurately describe a full-scale industrial process (Nadal-Rey et al., 2020).

As presented in Fig. 6, during its growth, \textit{Saccharomyces cerevisiae} performs three reactions: (i) the oxidation of glucose to biomass; (ii) the reduction of glucose to form biomass and ethanol; and (iii) the oxidation of ethanol to form biomass. In addition, the rate of oxygen dissolution in the medium is also included in the process model.

The metabolic reactions are mostly represented through Monod type equations, the most frequently used equations for bioprocess kinetics, with modifications for the regulatory and inhibitory effects (Table A1 Appendix A). The hypothesis is that the combination of the Monod equation with small modifications that represent common behaviours in bioprocesses (e.g., inhibition phenomena) could provide a good educational frame. Hence, each component of the model has to be explained. Once the model is properly characterized, it needs to be implemented, solved, and validated.

Step 2B.2: Model implementation

Implementation is, by definition, the realization or execution of an idea. Through model implementation, it is possible to encourage creative and practical learning by supporting a feeling of ownership and exploration. This has shown to be very beneficial in the act of applying high metacognitive levels of the Bloom’s taxonomy’s learning objectives.

In order to provide the educational frame for model implementation, the models are made available and explained to the students by providing: (i) Jupiter Notebooks; (ii) a GitHub model repository (https://github.com/simonetacannodelas/BioVL-Library); and, (iii) multimedia content. Additionally, an in-browser python code editor is currently being built into the software in order to enhance the implementation and the development of programming skills.

As previously mentioned, step 2 can be re-defined and adapted based on the inputs given by future users (refer to Fig. 2).

3.4. Step 3: Gamification design

The gamification strategy’s initial design is to place the students in a world where baking yeast is missing. Therefore, the gamification goal is to identify how to make baking yeast and how to optimize this process. This objective is then subdivided into a set of smaller goals, as presented in the skill tree developed for BioVL in Fig. 7.

In summary, the gamification strategy includes the elements of storytelling (for the action space), the introduction of goals, challenges, quizzes, positive and negative feedback, the possibility to choose different tasks, competition and cooperation.

It is important to highlight that the gamification design chosen is a user-centered design approach. This aims to ensure that the student’s needs are met and that the process simulator is understandable and usable (Norman, 2013). Thus, several user evaluation experiences must be performed and assessed for the successful development of the software.

3.5. Step 4: Participatory design of the process simulator

This step focuses on discovering the real issues related to what the students have experienced and what needs have not been met, not about finding solutions. However, the students “desired experience” highly depends on the group of undergraduate students; thus, several iterations may be necessary before converg-
Fig. 7. A hierarchical visual representation of customizations a student can make when using BioVL, the bioprocess simulator prototype developed in this work.

Fig. 8. Paper prototype for participatory design (de las Heras, 2018).

ing to the most satisfactory learning experience. Therefore, in this work, we present three iterations of the co-design process with various groups of students during different stages in the development of our process simulator. The objective of every new iteration is to gather ideas and suggestions on how to further improve BioVL since its design evolves and the number of features increases with each iteration. The first participatory design was performed during the conceptual design of the case study using a paper prototype (Fig. 8). Ten undergraduate students in the second year of their bachelor’s degree in sustainable biotechnology at the University of Aalborg (Denmark) participated and quantitative and qualitative information was collected in a guided process supported by a questionnaire (refer to Appendix B).

The quantitative data is represented in Fig. 9. This figure shows that approximately 60% of the participants asked for more information and clarification about the game objectives before playing. Therefore, the next iteration of the software required the reformulation of the set of rules in the gamification and in the learning design steps (see Fig. 11b for the next prototype iteration). Furthermore, the game storyline was changed, from a job interview to a particular scenario in which a microorganism needs to be cultivated and its growth is to be optimized. By using this new scenario, it is expected that the learning objectives are more limited and clearer. On the other hand, only 47% of the participants prioritized a more attractive interface over increasing the number of tasks inside the simulator (66%). Hence, the stu-
students/participants value the learning value of the simulator the most.

The qualitative information from this first experience focused on the initial stage of the process simulator’s design. The students engaged in an active conversation about the prototype and elaborated on how they would like to use it or how they would design it. For example, some of the student’s comments were “it might help on an exam or maybe for an oral presentation”, or “people like competitive games; maybe you could also make it more competitive for example adding multiplayer”. Based on the participants’ observations and positive feedback, BioVL was re-designed. One of the modifications done based on the inputs of the students is the decision to build BioVL as a web-based process simulator. This decision provides the users with a more accessible and multi-platform compatible system, and for example, it will later enable the designers to integrate online multiplayer features. This new version of the BioVL was then subjected to a second co-participatory experience with a new set of students.

The second participatory experience involved a session using a mock up inline software prototype (Fig. 10). Eight students from the undergraduate degree in biotechnology engineering at the University of Auckland, New Zealand, participated in the experience. A new strategy for the collection of data was used in this second co-participatory experience. This approach involved open conversations and discussion among the students and the developer. This strategy aimed to efficiently engage the students/participants to be more active and creative. Moreover, our intention with the new approach was to decrease the possible limitations of the questionnaire and reduce its biases.

After having tried the prototype, the participants criticized the lack of coding in their curriculum, and therefore, they highlighted that they would prefer to have more content about programming and model development in BioVL. The students also pointed out the presence of too much text (Fig. 11b) and bugs in the prototype. Hence, they gave suggestions on how to make the process simulator work smoother as well as suggestions on how to increase the content about model implementation (i.e., an integrated IDE with exercises).

Finally, a third co-participatory design experience has been performed using an online prototype of BioVL (Fig. 11), and suggestions for improvements were also collected by open conversation. This experience was done with only two students, due to the COVID-19 pandemic restrictions. These students were participating in the bioprocess technology course at the undergraduate degree from the Technical University of Denmark, Denmark.

In this case, the students asked for more explicit graphs and instructions on how to use the simulator, as well as more theoretical support on how to choose microorganisms. Besides, the students highlighted that the presence of pop-up windows was confusing and mostly unwanted. Based on these inputs, more information was included in the model library and the unnecessary pop-up windows were removed.

Currently, the updated version of the software will provide coding activities for agile learning by using a web-based IDE for python.

3.6. Step 5: Pedagogical verification

Finally, this last step aims to assess the suitability of the designed process simulator. To do so, three questionnaires have been developed to evaluate the perceived learning satisfaction and the usability and functionality of the graphical user interface. The perceived learning satisfaction questionnaire was developed using a reduced version of the methodology proposed in Nokelainen (2006). They have developed an empirical assessment of pedagogical usability criteria for digital learning material. Furthermore, the usability and functionality questionnaires also correspond to a selected part of previously developed surveys by Koretsky et al. (2011) and Harper and Norman (1993), respectively. Regarding learning satisfaction, we evaluate the applicability of the learning, the learner activity, and perceived usefulness of the students, and motivation. This assessment is based on the questionnaire developed for the assessment of pedagogical usability in digital learning (Nokelainen, 2006). Furthermore, the usability and functionality questionnaires focus on evaluating the weaknesses and strengths of the human-computer interactions. The questionnaires can be found in Table C1 (Appendix C), Table D1 (Appendix D), and Table E1 (Appendix E).

BioVL is still in its infancy, hence in the development stage. Consequently, the pedagogical validation has yet not been performed. In the future, the pedagogical verification can be done initially with small groups to identify the platform’s main issues, such as bugs, black screens or unsatisfactory content. Previous studies have found that 85% of usability and functionality problems that affect one in three users will be identified by using a group of five students (Nokelainen, 2006). However, for the evaluation of the learning satisfaction, a larger student group is here recommended.

3.7. Outcome: BioVL, an online educational bioprocess simulator

The outcome of applying the P2Si framework is the conceptual design of a process simulator prototype for the teaching of bioprocesses to undergraduate students (BioVL). The prototype of BioVL is available in www.bioVL.com.
Fig. 10. Inline mock-up software.

Fig. 11. Online software prototype.
It has been built as an open-source web-based simulator that includes the following features: (i) a library of bioprocess mathematical models in Python (also as a Github repository - https://github.com/simonetacanolas/BioVL-Library); (ii) multimedia resources for the explanation of the development of models and programming; (iii) introduction of disturbances inside the simulations to present more realistic scenarios; (iv) a chatbot for collaborative learning; (v) quizzes; (vi) the possibility to create "what if" scenarios by modifying the different parameters inside the model; and, (vii) the chance of troubleshooting the simulated bioprocess. 

Currently, we are performing iterations in the validation steps of the framework, so that the participation of the students in the design of the BioVL platform is fruitful and successful.

4. Conclusions

Education in engineering sciences faces challenges in continuing to provide high-quality, flexible, and updated learning in an ever-changing industrial world. Educational process simulators have shown to be an important tool to aid the instructors in the classroom and thus, help the students to acquire the knowledge and skills needed to complete the curriculum. This is especially valid in today's reality where on-line courses form an essential part of many curricula. Therefore, the proposed framework was designed to facilitate the development of such platforms. In essence, the P2Si framework provides a structured approach along with guidelines to explore the potential of modelling in the process systems education. Thus, P2Si leads the user to: (i) identify the necessary learning goal; (ii) construct the pedagogical description, and the mathematical development of process models following a hierarchical system; (iii) include a motivational strategy - in this case gamification; (iii); and actively involve the students as co-designers in a participatory experience. To demonstrate the applicability of P2Si, in this work we have developed a proof-of-concept in the form of a web-based educational bioprocess simulator (BioVL). BioVL is designed to be included in the Chemical and Biochemical Engineering undergraduate's curriculum. 

To conclude, we believe that designing targeted process simulators will help to prepare the students to have an active role in the transition to a more sustainable and digitalized reality, and thus become a pushing part of the Industry 4.0 movement.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Simona Caño de las Heras: Conceptualization, Methodology, Software, Investigation, Writing - original draft, Writing - review & editing. Carina L. Gargalo: Supervision, Methodology, Writing - original draft, Writing - review & editing. Charlotte Lærke Weitze: Resources, Writing - review & editing. Seyed Soheil Mansouri: Conceptualization, Funding acquisition, Writing - review & editing. Krist V. Gernaey: Supervision, Writing - review & editing. Ulrich Krühne: Supervision, Funding acquisition, Writing - review & editing.

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Appendix A. Kinetic model

Table A1

<table>
<thead>
<tr>
<th>Process</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxidative capacity of the cells ( r_C )</td>
<td>( r_C = \frac{\mu}{C_m} \cdot C_s ) ( \text{[A.1]} )</td>
</tr>
<tr>
<td>Glucose uptake rate ( r_C )</td>
<td>( r_C = qC \cdot \frac{C_G}{C_{t,0} - C_G} \cdot C_s ) ( \text{[A.2]} )</td>
</tr>
<tr>
<td>Product formation rate ( r_P )</td>
<td>( r_P = \frac{qP}{C_m} \cdot C_s ) ( \text{[A.3]} )</td>
</tr>
<tr>
<td>The oxidation rate of glucose ( (\mu_{Oxid,G}) )</td>
<td>( \mu_{Oxid,G} = Y_{Oxid} \cdot \frac{qC}{C_{t,0} - C_G} \cdot \frac{C_G}{C_{t,0} - C_G} \cdot Y_{GC} \cdot qC ) ( \text{[A.4]} )</td>
</tr>
<tr>
<td>The reduction rate of glucose ( (\mu_{Red,G}) )</td>
<td>( \mu_{Red,G} = \frac{Y_{Red,G}(C_G - \frac{qC}{C_{t,0} - C_G} \cdot \frac{C_G}{C_{t,0} - C_G} \cdot Y_{GC} \cdot qC \cdot \frac{C_{t,0} - C_G}{C_{t,0} - C_G} \cdot Y_{GC} \cdot qC ) ( \text{[A.5]} )</td>
</tr>
<tr>
<td>The oxidation rate of ethanol ( (\mu_{Oxid,E}) )</td>
<td>( \mu_{Oxid,E} = \frac{qE}{C_{t,0} - C_E} \cdot Y_{OE} \cdot \frac{C_E}{C_{t,0} - C_E} \cdot Y_{GC} \cdot qC ) ( \text{[A.6]} )</td>
</tr>
<tr>
<td>Biomass growth rate</td>
<td>( \mu = \mu_{Oxid,G} + \mu_{Red,G} + \mu_{Oxid,E} ) ( \text{[A.7]} )</td>
</tr>
<tr>
<td>Oxygen supply</td>
<td>( k_3 \cdot (C_{O_2} - C_{O_2}) ) ( \text{[A.8]} )</td>
</tr>
</tbody>
</table>
Appendix B. Survey for the first co-participatory experience

Section for Sustainable Biotechnology
Department of Chemistry
and Bioscience Aalborg
University Copenhagen

Questionnaire for the test of the paper prototype 29/11/2017

Please, qualified the questions from totally agree (2), agree (1), neutral (0), disagree (-1) or totally disagree (-2).

1. Do you think this tool could help you learning about a specific fermentation?

Could you explain with your own words how the tool helps/doesn’t help you in learning about fermentation? Please give one or two examples...

2. Do you like the idea of gamification (using some things from games) for studying?

3. Do you think you could extrapolate the knowledge to a “hand-on” process?

Could you explain with your own words how the tool helps/doesn’t help you in an extrapolation of theory into actual fermentation? Please give one or two examples...

4. Do you consider the content easy?

If you agree or strongly agree, could you help us to increase the level?

5. Do you like the feedback?

(for example; Congratulations, you are rocking it) Please give one or two examples of why do you like it or not...
Appendix C. Learning verification

Table C1

<table>
<thead>
<tr>
<th>Statement in the questionnaire</th>
<th>Pedagogical domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>I’m interested in the topic of this learning material.</td>
<td>Meaningful encoding</td>
</tr>
<tr>
<td>This learning material presents new material in “portions” suitable for me.</td>
<td>Meaning encoding in learning applicability</td>
</tr>
<tr>
<td>When I work in this learning material, I have to find out my solutions without the instructor’s or the program’s model solutions.</td>
<td>Problem-based learning</td>
</tr>
<tr>
<td>This learning material provides learning problems without a pre-defined model for solutions.</td>
<td>Problem-based learning</td>
</tr>
<tr>
<td>I feel that I will be able to use the skills and knowledge this software has taught me in the future.</td>
<td>Perceived usefulness</td>
</tr>
<tr>
<td>The learning material is strictly limited.</td>
<td>Learning control over their learning</td>
</tr>
</tbody>
</table>

Appendix D. Usability

Table D1

<table>
<thead>
<tr>
<th>Statement in the questionnaire</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 What do you think the instructors intended you to learn by using the software?</td>
</tr>
<tr>
<td>2 How would you explain the software to a first-year student?</td>
</tr>
<tr>
<td>3 When you close your eyes and picture the software, what do you see? (e.g. when I close my eyes and imagine Skype business, I see a black screen with a lot of squares. I can send some emojis and I like to be able to have a chat. However, I don’t see a lot of differences with Zoom or Team.</td>
</tr>
</tbody>
</table>

Appendix E. Functionality

Table E1

<table>
<thead>
<tr>
<th>Statement in the questionnaire</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Rate the use of the software from terrible (0) to wonderful (10)</td>
</tr>
<tr>
<td>2 Rate the use of the software from difficult (0) to easy (10)</td>
</tr>
<tr>
<td>3 Rate the use of the software from frustrating (0) to satisfying (10)</td>
</tr>
<tr>
<td>4 Rate the use of the software from dull (0) to stimulating (10)</td>
</tr>
<tr>
<td>5 Rate the use of the software from rigid (0) to flexible (10)</td>
</tr>
</tbody>
</table>

References
