

Immersive Technologies with Computational Fluid Dynamics in Engineering Education

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Preface

Questioning is one of the first skills I was aware of when I came to know myself. My curiosity always keeps me alive to actively seek understanding of my presence. We have so little time in this finite existence but have a lot to learn and create. Over the years, fluid dynamics has become a central part of my curiosity due to its sophisticated but startling nature. The deeper I have got, the more intriguing it has become. I am obviously not the only one amazed by the astonishing nature of fluid dynamics. In the 17th century, Leonardo da Vinci devoted a part of his life and curiosity to untwisting its chaotic characteristic. It takes only a second to get you perplexed by his legacy when you take a glance at his codex; a truly remarkable artist, scientist and engineer, of course among many others who may have somehow gotten into this rabbit hole but did not unfortunately leave any artifacts that we today know of. Having eventually landed on this doctoral study, I have spent four intriguing years broadening my analytical, critical and emotional thinking whereas intrinsically practicing Socratic questioning and critical thinking. I therefore wholeheartedly dedicate this thesis to all curious minds questioning our existence to provide a better life for living beings.

I am writing this preface to express my deepest gratitude and appreciation for the support and guidance that I received throughout this non-linear journey, especially from the ones that helped me grow intellectually and emotionally.

First of all, I would like to express my deepest appreciation to my supervisor Prof. Tom Van Gerven for his encouragement, advice, and belief in me have been invaluable and have played a crucial role in helping me to successfully end up my doctoral research. "A Ph.D. is constantly looking for ways", this was what you told me when I was struggling with the formulation of my research question. Your encouragement and belief in me meant so much, especially during the challenging times. Your support, guidance and overall insights in this field have genuinely made this an inspiring experience for me.

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I have met countless amazing people from all over the planet Earth; Turkey, Italy, Romania, South Korea, China, Iran, Greece, the USA and any other countries that you can name. Thank you all for consciously or not helping me to become what I am today, as well as playing a decisive role in my decisions. I am genuinely grateful to have you in my life.

Lastly, I would also like to extend my deepest appreciation to my family and beloved ones to express my heartfelt gratitude for their unwavering support.

It was a long and challenging process, and I could not have done it without your love and support. Laetitia, thank you for unconditionally believing in me and always being there for me from the very beginning, which greatly helped me to stay focused and keep my mental well-being good. Also thank you for being a great mother to our lovely daughter. Emma, you joined us in March 2022 the last year of this journey. I am now more resilient than ever with you owing to the first three sleepless months. Thank you for being a lifeline for me with your endless smiles. I have already compiled a long to-do list to show you how amazing the world we live in is. Just looking forward to the moments when I can teach and learn from you. I also would like to thank my family; my mother, father and brother. Their belief in me, encouragement and love have meant the world to me and have helped me to persevere through the challenges and setbacks that inevitably arise during the research process. Thank you for everything, and for being my inspiration to be the best that I can be.

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Abstract

Learning is a cognitive process to acquire and store new information and retrieve it when needed. Knowledge, skills, values and concepts are basic forms of information that the human brain can learn. The human brain is one of the utmost complex organs that humankind tries so hard to theorize its functionalities. What we know to date is that despite its uniqueness, the brain has a limited capacity to process new information. This does not mean that the brain cannot learn everything. In contrast, the brain has an exclusive ability to explicate the most challenging things that humankind is somehow aware of, but it has its own rules and processes to make learning happen.

Still, this limited capacity has discovered and created every piece of information that today exists, or once existed. Notably, today's engineering design tackles complex problems to provide efficient solutions for a sustainable world. Engineering problems have become intricate and require interdisciplinary approaches to unveil novel solutions. Teaching and communicating these problems may even get more complex since such practices require great effort to produce adequate learning materials and practices. In particular, chemical engineering has put great effort into pushing the boundaries toward efficiency and sustainability. Mixing, for example, is one of the core unit operations in chemical engineering taking part in almost every chemical process. In particular, in order to develop an ultrasound-assisted milli-fluidic crystallizer to produce pharmaceuticals efficiently, an engineering student should be able to comprehend and interpret transport phenomena, acoustics, multiscale and multiphysics interactions. Not only handbook solutions and experimental studies, but also multiphysics computational fluid dynamics (CFD) simulations are blended into the technical work to make progress in an efficient and effective manner.

CFD simulations are essential tools to support engineering design and analysis. Cost time benefits, advanced data visualization and virtual prototyping are the main advantages of CFD simulations. A deep understanding of physical, mathematical and computer science is critical to obtain reliable simulation

projects. These require physical accuracy, optimal calculation time and meaningful result extraction. CFD simulations have a dynamic role to play in engineering education; producing abstract learner content and facilitating active learning environments. However, computationally demanding data production and complex data processing environments of CFD simulations turn them into esoteric tools for potential non-expert users. Neither lecturers nor students may have acquired the relevant skills to deal with the complex nature of simulation environments. The application and communication of CFD simulations in engineering education is consequently limited.

Technology is the driver of 21st-century education. Augmented reality (AR) and virtual reality (VR) are immersive technologies that have recently been receiving much attention due to the advanced levels of immersion and interaction on cognitive, affective and behavioral domains. Immersive technologies with CFD simulations have been studied by a limited number of researchers in an attempt to find a new dimension in the utilization of CFD in engineering education. Nevertheless, little is known about the integration of CFD simulations with immersive technologies in engineering education, and it is not clear how to design, develop, evaluate and implement such learning environments. The ultimate goal of this dissertation is to broaden our understanding of immersive technologies with CFD simulations in engineering education.

A systemic approach is not available on how to integrate CFD data into game engines to develop AR/VR applications. All the previously mentioned methods suffer from serious limitations due to highly specific software components. Therefore, we initially aim at developing a system architecture to picture a state of cross-platform integration. The following step explores potential data processing workflows to disclose feasible solutions using an extract-based data processing approach. A modular data processing pipeline is established upon lightweight, open-source and automated components. Our approach enables an inclusive workflow that non-experts can easily pursue to integrate intended CFD data in AR/VR software.

As a relatively new research dimension, immersive technologies with CFD simulations are generally developed to examine both technical and psychological factors with standalone, non-interactive and offline AR/VR applications with CFD data. Despite the popularity of connected and sustainable software systems to achieve long-lasting solutions, it is likely that there is a strict need for experts to maintain a dynamic data flow between CFD solvers and AR/VR applications. A possible explanation for this may be the lack of adequate middleware and expertise to uncover a dynamic connection. Immersive and portable user devices dramatically suffer from the computational power that is required to deal with intensive numerical calculations in CFD simulations. A reasonable approach to tackle this issue can be to remotely deliver CFD content to immersive devices.

In the second step of this research, we introduce a client-server architecture with a fully automated routine, enabling a two-way connection between CFD solvers and AR/VR applications. Workflows comprising both open-source and commercial products are established and quantitatively assessed highlighting advantages and pitfalls. In addition, we introduce an educational VR concept with custom human-centric tools to properly interact with CFD simulations.

A VR prototype, namely the Virtual Garage, is developed to educate engineering students about real-life engineering problems to be solved using CFD simulations. A feasibility study is carried out in advance to pinpoint contents that matter in the chemical engineering curriculum. Learning materials and environment are designed in light of available pedagogical guidelines. We perform two sets of experiments to validate our design and assess its value in engineering education. In the first step, users ($n=24$) evaluate the VR prototype by means of usability, user experience, task load and simulator sickness within a mixed methodology. Results are further correlated to draw logical conclusions upon user experience and interest in content and technology. The Virtual Garage is well-received by users. We identify features that can further leverage the quality of the immersive learning environment with CFD simulations. In the second step, we evaluate behavioral intention to use the Virtual Garage, as well as perception before and after intervention ($n=57$). Results indicate that the learning value, content value, intrinsic motivation and personal innovativeness are underlying factors behind students' intention to use the Virtual Garage. The pair-wise analysis points out that users' perception matter and positively affect their attitudes. In an attempt to assess learning in a pair-wise comparison, it is revealed that users perform significantly better in the post-knowledge test, and this is accordingly reflected in task performance.

In conclusion, the educational use of immersive technologies with CFD simulations shows the potential of immersive learning to reduce the entry barrier for complex engineering concepts. We discuss the implication of the findings to future research in this area.

Beknopte samenvatting

Leren is een cognitief proces om nieuwe kennis te verwerven en verwerken. Kennis, vaardigheden, waarden en concepten zijn basisvormen van informatie die het menselijk brein kan leren. Het menselijk brein is een van de meest complexe organen die de mensheid tracht te doorgronden en de functionaliteiten ervan te theoretiseren. Wat we tot nu toe weten, is dat het brein, ondanks zijn uniekheid, een beperkt vermogen heeft om nieuwe informatie te leren. Dit betekent echter niet dat de hersenen niet alles kunnen leren. Het brein heeft het exclusieve vermogen om de meest uitdagende dingen te verklaren waarvan de mensheid zich op de een of andere manier bewust is, maar het heeft zijn eigen regels en processen om leren mogelijk te maken.

Desalniettemin heeft deze beperkte capaciteit elk stukje informatie ontdekt en gecreëerd dat vandaag bestaat, of ooit heeft bestaan. Met name de hedendaagse en vaak hoogtechnologische innovaties staan toe complexe problemen aan te pakken zodoende efficiënte oplossingen te bieden voor een duurzame wereld. Technische problemen worden alsmaar ingewikkelder en vereisen interdisciplinaire benaderingen om tot nieuwe oplossingen te komen. Het onderwijzen en communiceren van deze problemen kan zelfs nog complexer worden, daar dergelijke praktijken veel inspanning vergen om adequaat leermateriaal en geschikte praktijken te produceren. Vooral de chemische technologie heeft veel energie gestoken in het verleggen van de grenzen naar efficiëntie en duurzaamheid. Mengen is bijvoorbeeld een van de kernactiviteiten in de chemische technologie die terugkomt in quasi elk chemisch proces. Om bijvoorbeeld een door ultrageluid ondersteunde millikristallisator voor de efficiënte productie van geneesmiddelen te ontwikkelen, dient men te beschikken over enige notie omtrent transportverschijnselen, akoestiek en andere fysische interacties die kunnen plaatsvinden op verschillende tijd- en lengteschalen. Niet alleen handboekoplossingen en experimentele studies, maar ook numerieke stromingsleer kan hierbij worden toegepast als hulpmiddel.

Numerieke stromingsleer (Engels: Computational Fluid Dynamics of CFD)

zijn tegenwoordig onmisbaar ter ondersteuning van technisch ontwerp en analyse. Het verminderen van de algemene kost en ontwikkelingstijd, geavanceerde datavisualisatie en virtuele prototyping zijn de belangrijkste voordelen van CFD-simulaties. Inzicht in natuurkundige en wiskundige begrippen uit de stromingsleer, evenals kennis van informatica, is hierbij van cruciaal belang om tot optimale simulatieworkflows te komen. Deze vereisen fysieke nauwkeurigheid, optimale rekentijd en zinvolle extractie van resultaten. CFD-simulaties spelen een dynamische rol in technisch onderwijs, door abstracte leerinhoud te produceren en actieve leeromgevingen te faciliteren. Echter, computationeel veeleisende dataproduktie en complexe dataverwerkingsomgevingen van CFD-simulaties veranderen ze in esoterische hulpmiddelen voor potentiële niet-deskundige gebruikers. Noch docenten, noch studenten hebben mogelijk de relevante vaardigheden verworven om met de complexe aard van simulatieomgevingen om te gaan. Dit beperkt bijgevolg de toepassing en communicatie van CFD-simulaties in het technisch onderwijs.

Technologie is de motor van het onderwijs van de 21e eeuw. Aangevulde realiteit (Engels: augmented reality of AR) en virtuele realiteit (Engels: virtual reality of VR) zijn immersieve technologieën die de laatste tijd veel aandacht hebben gekregen vanwege de geavanceerde niveaus van immersie en interactie op cognitief, gedrags- en emotioneel niveau. Immersieve technologieën met CFD-simulaties zijn door een beperkt aantal onderzoekers bestudeerd in een poging een nieuwe dimensie te vinden in het gebruik van CFD in technisch onderwijs. Desalniettemin is er weinig bekend over de integratie van CFD-simulaties met immersieve technologieën voor onderwijsdoeleinden en is het niet duidelijk hoe dergelijke systemen moeten worden ontworpen, ontwikkeld, geëvalueerd en geïmplementeerd. Het uiteindelijke doel van dit proefschrift is om ons begrip van immersieve technologieën te verbreden met CFD-simulaties in het technisch onderwijs.

Er is geen systematische benadering beschikbaar voor het integreren van CFD-gegevens in game-engines om AR/VR-toepassingen te ontwikkelen. Alle eerder genoemde methoden hebben aanzienlijke beperkingen vanwege zeer specifiek mechanismen. Daarom richten we ons in eerste instantie op het ontwikkelen van een systeemarchitectuur om een beeld te schetsen van een staat van platformafhankelijke integratie. De volgende stap onderzoekt mogelijke werkstromen voor gegevensverwerking zodoende haalbare oplossingen aan te bieden met behulp van een op extracten gebaseerde benadering voor gegevensverwerking. Er wordt een modulaire pijplijn voor gegevensverwerking opgezet op basis van lichtgewicht, open-source en geautomatiseerde componenten. Onze aanpak maakt een inclusieve workflow mogelijk die leken gemakkelijk kunnen nastreven om beoogde CFD-gegevens in AR/VR-software te integreren.

Als relatief nieuwe onderzoeksdimensie worden immersieve technologieën

met CFD-simulaties over het algemeen ontwikkeld om zowel technische als psychologische factoren te onderzoeken met stand-alone, niet-interactieve en offline AR/VR-toepassingen met CFD-gegevens. Ondanks de populariteit van verbonden en duurzame softwaresystemen om duurzame oplossingen te bereiken, is het waarschijnlijk dat er een strikte behoefte is aan experts om een dynamische gegevensstroom tussen numerieke methodes en AR/VR-toepassingen te onderhouden. Een mogelijke verklaring hiervoor is het ontbreken van adequate middleware en expertise om een dynamische verbinding bloot te leggen. Draagbare gebruikersapparaten hebben drastisch te lijden onder de verhoogde rekenkracht die nodig is om intensieve numerieke berekeningen uit te voeren. Een redelijke benadering om dit probleem aan te pakken, kan zijn om CFD-gegevens op afstand te leveren aan immersieve apparaten. In de tweede stap van dit onderzoek introduceren we een client-server-architectuur met een volledig geautomatiseerde routine, waardoor een tweerichtingsverbinding tussen CFD-solvers en AR/VR-applicaties mogelijk is. Workflows die zowel open source als commerciële producten omvatten, worden gevormd en kwantitatief beoordeeld, waarbij de voordelen en valkuilen worden benadrukt. Daarnaast introduceren we een educatief VR-concept met aangepaste mensgerichte tools om goed te kunnen communiceren met CFD-simulaties.

Een VR-prototype, genaamde de Virtuel Garage, is ontwikkeld om technische studenten kennis te laten maken met echte technische problemen. Er wordt vooraf een haalbaarheidsstudie uitgevoerd om de relevantie en toepasbaarheid binnen het curriculum van de chemische technologie af te toesten. Het leermateriaal en de omgeving zijn ontworpen in het kader van de beschikbare pedagogische richtlijnen. We voeren twee reeksen experimenten uit om ons ontwerp te valideren en de waarde ervan in het technisch onderwijs te beoordelen. In de eerste stap evalueren gebruikers ($n=24$) het VR-prototype op basis van gebruiksvriendelijk en - ervaring. De resultaten worden gecorreleerd om logische conclusies te trekken op basis van de ervaring en interesse van gebruikers. De Virtuel Garage wordt goed ontvangen door gebruikers. We identificeren functies die de kwaliteit van de leeromgeving verder kunnen benutten met CFD-simulaties. In de tweede stap evalueren we de gedragsintentie van gebruikers om de Virtuel Garage te gebruiken, evenals hun perceptie voor en na blootstelling ($n=57$). Resultaten geven aan dat de leerwaarde, inhoudswaarde, intrinsieke motivatie en persoonlijke innovativiteit onderliggende factoren zijn achter de intentie van studenten om de Virtuel Garage te gebruiken. De paarsgewijze analyse wijst erop dat de perceptie van gebruikers ertoe doet en hun houding positief beïnvloedt. In een poging om leren te beoordelen in een paarsgewijze vergelijking, is gebleken dat gebruikers significant beter presteren in de post-kennistest, en dit wordt weerspiegeld in taakprestaties.

Gelet deze resultaten, kan er worden geconcludeerd dat het educatieve gebruik

van immersieve technologieën met CFD-simulaties het potentieel aantoont van immersive learning om de toegangsdrempel voor complexe technische concepten te verminderen. We bespreken de implicatie van de bevindingen voor toekomstig onderzoek op dit gebied.

List of Abbreviations

4C/ID	Four-component instructional design
ADDIE	Analysis, design, development, implementation and evaluation
AI	Artificial intelligence
API	Application programming interface
AR	Augmented reality
AVE	Average variance extracted
AWS	Amozon web service
CAD	Computer aided design
CAE	Computer aided engineering
CDN	Content delivery network
CFD	Computational fluid dynamics
CLT	Cognitive load theory
CPU	Central processing units
CV	Content value
DoF	Degree of freedom
EE	Effort expectancy
FMI	Functional mock-up interface
FT	Flow theory
GLB	Game based learning
GPS	Global Positioning System
GPU	Graphical programming units
GUI	Graphical user interface
H	Habit
HCI	Human computer interaction
HMD	Head mounted display

HPC	Human computer interaction
HTMT	Heterotrait monotrait ratio
IBL	Inquiry-based learning
ICT	Information and communication technology
IoT	Internet of things
IV	Intrinsic value
LV	Learning value
MR	Mixed reality
NASA-TLX	NASA task load index
NURBS	Non-uniform rational b-splines
OST	Optical see through
PE	Performance expectancy
PI	Personal innovativeness
PLS-SEM	Partial least squares structural equation modeling
ROM	Reduced order model
SAMR	Substitution augmentation modification redefinition
SDK	Software development kit
SE	Self-efficacy
SSQ	Simulator sickness questionnaire
SUS	System usability scale
TAM	Technology acceptance model
TOE	Technology organization environment
TPACK	Technological pedagogical content knowledge
UEQ	User experience questionnaire
UTAUT	Unified theory of acceptance and use of technology
VIF	Varience inflation factor
VR	Virtual reality
VST	Video see through

List of Publications

Journal articles (peer-reviewed)

Solmaz, S., & Van Gerven, T. (2021). Automated integration of extract-based CFD results with AR/VR in engineering education for practitioners. *Multimedia Tools and Applications*, 81(11), 14869-14891. <https://doi.org/10.1007/s11042-021-10621-9>

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Chapter 1

Introduction

Since the turn of the 2000s, technology has become ubiquitous, a core element of our life in engineering and education. It was in the early 1900s when the first known instructional videos were produced [1]. It took some 60 years to ideate and prototype the first virtual reality (VR) experience. French playwright Antonin Artaud named the concept first time in literature “la réalité virtuelle” defining unusual features of characters in a theater [2]. In general terms, VR is a digital environment in which users are cognitively and physically immersed through sensory stimuli. Depending on the fidelity of the application, it could be very similar to real-life experiences, even more leveraged by adapting advanced features of technology to stimulate immersion, interaction and presence. Likewise, augmented reality (AR) and mixed reality (MR) are variations of VR combining the real environment with digital content. All these digital technologies are commonly referred to as immersive technologies due to triggered sensory stimuli, surrounding individuals physically and cognitively. Over the last decade, there has been a revolution in immersive technologies making them progressively accessible and affordable for educational use [3]. The immersive technology market is expected to reach USD 87 billion by 2030, while it was only USD 11 billion in 2020 [4].

Technology has gradually transformed education, and will undoubtedly become the main driver of educational practices in 10 to 15 years [5]. In the new digitalized era, immersive technologies have been commonly applied to provide complementary and supplementary tools for learners. Notably, immersive technologies in education have been increasingly researched to uncover cognitive, affective and behavioral aspects of digital experiences [6]. Immersive learning, which has become a prominent branch of education, is a

digital experience that can involve immersive technologies to simulate real-life scenarios and educate learners in an effective, cheap and safe manner [7]. The European Union has released several research plans to adopt digital resources in education and training, including a recently published Digital Education Action Plan for 2021–2027 [8]. The plans envision concrete steps to lead to a high-performing digital education ecosystem with digitally competent human resources. Principally, high-quality learning content and user-friendly tools have been strictly underlined together with the emergence of immersive technologies.

In the early 1920s, Lewis Fry Richardson was doing hand calculations to carry out weather forecasts when computers did not yet exist. He once claimed that 60,000 individuals would be needed to predict tomorrow's weather before it came [9]. It was only in the 1940s when computers such as ENIAC were developed to perform numerical analysis to solve fluid dynamics problems [10]. Computational fluid dynamics (CFD) is a physics-based numerical tool to predict solutions for problems comprising fluid flow and relevant physical and chemical phenomena. It has been widely adopted in industry and academia as being a cost time effective support and alternative to physical experiments. Preparation, calculation, and post-processing are a set of subsequent steps that are executed manually by a competent analyst. CFD simulation results are generally analyzed in a heavily interactive process with specialized post-processing software to obtain meaningful data in support of modeling, design and decision-making. A deep understanding of physical, mathematical and computer science is critical to obtain optimal simulation workflows. Thanks to the recent and continuous advancements in computer science and mathematics, computational power has been groundbreaking increased, thus enabling a paradigm shift in computation. As of today, it is possible to perform real-time CFD simulations with simplified models and data-driven setups. Personal computers can even be employed to perform CFD simulations for varying degrees of accuracy. Nevertheless, the educational use of CFD simulations has been practiced with a limited capacity because of the expertise required in CFD software and computer graphics. A paradigm shift is essential to unlocking the potential of CFD simulations in education and training.

1.1 Problem statement

Applied engineering deals with complex problems to provide efficient solutions for a sustainable world. As a consequence, engineering problems have become intricate and require interdisciplinary approaches to unveil novel solutions [11]. Teaching and communicating these problems may even get more complex since such practices require great effort to produce adequate learning materials.

Policymakers have been addressing digital education to encourage a paradigm shift in education with high-quality, inclusive and sustainable tools [8]. Notably, CFD simulations are heavily applied in engineering design and analysis in support of decision-making. The use of simulation tools in engineering education is also getting prominent to provide required technical skills and also competencies such as critical thinking, decision-making, problem-solving, as well as advanced spatial reasoning skills [12]. CFD simulations have a dynamic role to play in engineering education to prepare students for real-life settings while boosting their understanding of complex engineering methodologies.

The educational use of CFD has two sides. While CFD simulations can provide accurate educational content to design learning experiences with easy-to-comprehend visualizations, they can also be utilized as computational tools to dynamically produce data and operate active learning environments. The latter is generally integrated into course projects to get students familiar with CFD methodology and software. Yet, computationally demanding data production and complex data processing environments of CFD simulations turn them into esoteric tools for non-expert users. Engineering students can face a high entry barrier in simulation environments developed through conventional simulation workflows such as using commercial CFD software with 2D desktop settings. In addition, CFD simulation data can be utilized in the existing educational context in the form of video clips and images. However, in such practices, students cannot directly interact with simulation data, thereby merely experiencing a passive participation. Lecturers should also provide sufficient supportive information to help students understand the basics of the problem solved by CFD simulations. Neither lecturers nor course developers might have acquired relevant skills to deal with the complex nature of CFD simulation and post-processing software to create user-friendly educational applications. These can hinder the utilization of CFD simulations and simulation data in education in an effective and interactive manner. Students may not properly grasp the content and context, as well as the methodology of CFD simulations in engineering.

Immersive technologies have recently been receiving much attention due to the advanced levels of immersion, interaction and presence [6, 13, 14]. Immersive learning environments may reduce the entry barrier to cognitively complex learning subjects [15]. These environments can positively trigger cognitive skills with advanced spatial interactions and easy-to-access technical content, as well as affective and behavioral aspects of learning such as motivating students to adopt new educational technologies [6]. This might open gates for user-friendly, high-quality complex learning environments assisted with CFD simulations that can be readily operated by students. Nonetheless, a huge gap is still present in the literature on the design, development, evaluation and implementation of immersive learning tools with CFD simulations [16, 17]. The adaptation

of AR/VR, particularly in engineering education, is facing a stiff challenge due to lacking relevant digital content, and more broadly, missing reliable guidelines in the design, development, evaluation and implementation of such tools [13, 18, 19, 20, 15, 21].

Integration of CFD data into AR/VR software

AR/VR technologies with CFD simulations have been proposed in a series of studies to prevail over the shortcomings of traditional simulation environments [22, 23, 24, 25]. However, many research questions are still posed on the technical content, infrastructure, accessibility, affordability, operability, and portability of digital resources [26, 27]. Essentially, arbitrary development methodologies of AR/VR tools have generally resulted in single-use digital environments rather than long-lasting sustainable applications [27, 28]. The integration of CFD results with AR/VR recently received scholarly attention. Literature is still missing a methodology and data integration process to guide the practitioners [16]. In addition, platform-specific, computationally-demanding, non-replicable and manual integration methodologies have mostly been reported by researchers [16, 17]. A conclusion has still not been drawn on how to post-process big CFD data into manageable parts, which an AR/VR development platform and end-user devices can handle. Additionally, no study has been reported on the multiplatform integrity to assess the data processing performance through data format, size, processing time, quality, automation and management. These ambiguities prevent practitioners to utilize AR/VR tools to visualize CFD simulation data [16, 17].

Sustainable immersive technology ecosystem with CFD simulations

Integration of CFD simulation data with AR/VR has already been studied and received positive feedback from early users [29, 16, 17]. Despite this, studies tended to focus on the domain- and platform-specific applications with non-replicable elements in their systems, thereby posing a danger to be outdated in a short period of time. Digital applications are generally hardcoded, offline and standalone, comprising a static CFD post-processing without any connection to a CFD solver or data processor [16]. Technical integration of simulation data with cross-platform software is still to be studied to obtain long-lasting sustainable digital applications concerning software development workflows, remote connection, automation, data visualization, human-computer interaction (HCI) and user evaluation [17]. Above all, manual expert interferences are still highly required in most cases to automate data generation and simulation routines [30, 31, 32, 33, 34]. There is still considerable ambiguity to maintain a sustainable software architecture between commonly used CFD solvers and AR/VR software.

Design and evaluation of user applications

Several proofs-of-concept have been demonstrated in immersive technologies to educate non-experts with CFD data such as engineering students [35], medical experts [36] and farmers [37]. Developing VR environments with physics-based high-fidelity engineering calculations can create value to provide high-quality immersive and interactive educational tools [19]. Visualization of CFD data in VR can enable a better interface than 2D screens to work with complex datasets in the context of scientific visualization [38]. In addition, given the complexity of the CFD workflow and methodology, immersive visualization of CFD simulations in AR/VR is not yet sufficient for non-experts. The learning environment should be adequately structured considering relevant components of pedagogy and instructional design. However, studies tend to overlook the added value of pedagogy since the research is still mostly dominated by technical challenges. Likewise, only a few researchers have assessed digital products with relevant metrics and target users. It appears that more research on the evaluation of applications and user assessments is essential to provide better immersive learning experiences and unlock the potential of these tools from students to policymakers [16, 17, 39, 40].

1.2 Scope of the thesis

The research presented in this dissertation was performed in the context of the European Training Network for Chemical Engineering Immersive Learning (CHARMING) which received funding from the European Union's EU Framework Program for Research and Innovation Horizon 2020 under Grant Agreement 812716. CHARMING is an interdisciplinary project aiming to study the implementation of immersive learning techniques in chemistry and chemical engineering education. The project consists of 15 doctoral researchers from three work packages focusing on children, high school and university students, and employees of the chemical industry. Engineers, educational scientists and game developers form a diverse competent human resource to achieve the multidisciplinary objectives of the project.

The purpose of this thesis is to investigate the potential of multiphysics CFD simulations with immersive technologies in chemical engineering education. The thesis does not engage with the education of CFD software and relevant competencies such as coding, geometry preparation, numerical methods and so forth; which is clearly beyond the scope of this thesis.

The research targets the design, development and assessment of user-friendly digital immersive learning applications with CFD simulations to teach complex

engineering subjects in chemical engineering such as intensified mixing processes. The central question in this dissertation asks how CFD simulations in immersive technologies can help reduce the entry barrier to complex engineering concepts with immersive learning while boosting cognitive, affective and behavioral domains. The ultimate objectives of the present research are:

- to apply CFD models and databases for chemical-model-based AR/VR design;
- to develop immersive learning concepts and prototypes with AR/VR technologies for intensified mixing processes;
- to translate the design and operating principles of intensified reactors into immersive learning concepts with AR/VR technologies;
- to assess the integrity of and promote guidelines for reactor models with CFD simulations in immersive learning environments with AR/VR technologies.

1.3 Outline

This thesis is composed of an introduction, a state-of-the-art, four main research chapters, a conclusion and perspectives, and an appendix with supplementary information at the end.

Chapter 2 elaborates on the state-of-the-art describing pillars of the methodology utilized to achieve research objectives under the umbrella of immersive learning: CFD, pedagogy and immersive technologies.

In Chapter 3, we introduce a system architecture and data processing pipeline to integrate CFD simulation data into game engines as cross-platform AR/VR development tools. Our goal is to fundamentally enable a simple, optimized, replicable and open-source data processing methodology that enthusiasts can readily integrate CFD data into AR/VR hardware and software.

In Chapter 4, a software architecture is proposed and discussed to develop an automated connection between CFD solvers and the Unity game engine to perform interactive simulations. The performance of the connection is quantitatively analyzed using both commercial and open-source CFD software. We further elaborate on CFD-specific software features to adequately interact with CFD simulations in VR, as well as on high-fidelity digital twins with physics-based models.

In Chapter 5, we conceptualize an immersive learning environment with CFD simulations in VR and develop a prototype. A user study is performed to

evaluate usability, user experience, task load and simulator sickness by applying a mixed methodology. We assess the validity of design guidelines and obtain potential improvements to facilitate a better immersive learning experience with CFD simulation for learners.

In Chapter 6, a technology acceptance model is proposed and assessed to predict underlying factors behind the behavioral intention to use an immersive virtual reality environment with CFD simulations. Perception and user performance are additionally studied to explore the potential implementation of similar tools in current educational practices. We identify substantial implications that can help developers and lecturer come up with desired immersive learning experiences with CFD simulations.

Chapter 7 draws general conclusions with future perspectives. In final, the appendix provides the supplementary information for each chapter.

Chapter 2

State-of-the-art

2.1 Introduction

Immersive technologies are rapidly becoming a key enabler in the digitalization of the educational ecosystem [6, 41]. A number of theoretical frameworks have long been released to integrate technology into education. Technology-Organization-Environment (TOE) is one of the forerunners implementing technological innovations concerning organizational and environmental factors [42].

From an educational point of view, a well-known example is introduced by Wasson et al. to enhance the learning environment with technology considering an interplay among three main dimensions: institution, pedagogy and technology [43]. In particular, Technological Pedagogical Content Knowledge (TPACK) [44] and Substitution-Augmentation-Modification-Redefinition (SAMR) [45] have recently received much attention to benefit from recent technological advancements to increase the quality of learning environments. TPACK proposes an approach to ease the implementation of technology in education with relevant content; whereas SAMR enables a modular approach to enhance and transform educational materials into meaningful digital assets, as can be seen in Fig. 2.1. These frameworks show that the development and sustainability of digital educational environments are strongly related to interdisciplinary skills from engineering, informatics and educational science.

Current educational practices provide very limited interaction with multiphysics CFD simulations and hinder its potential due to technological challenges and pedagogical ambiguities [16, 17]. Immersive technologies and pedagogical design tools can unlock the potential of CFD simulation in engineering education. Yet,

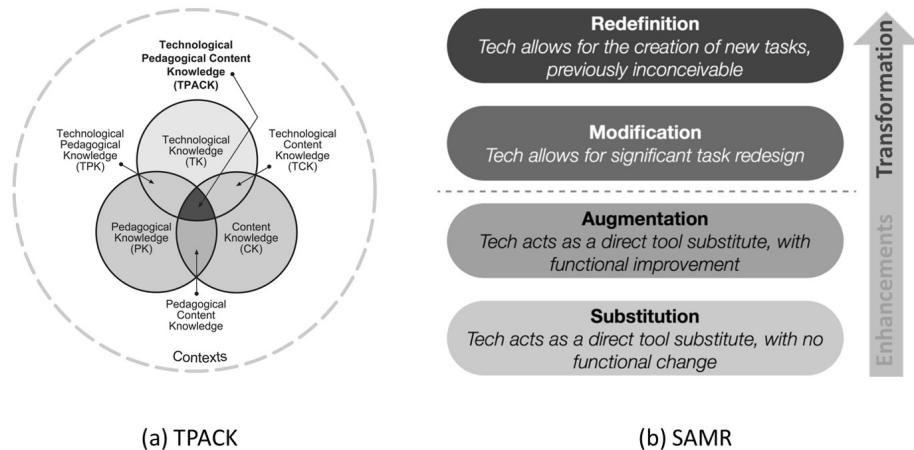


Figure 2.1: Technological Pedagogical Content Knowledge (TPACK) (a); Substitution-Augmentation-Modification-Redefinition (SAMR) (b).

there are several questions that remain unanswered about how CFD simulations can be adequately utilized with immersive technologies and relevant pedagogical guidelines to become a part of sustainable digitalization in education.

The following sections demonstrate the current state of the knowledge that serves as a foundation for our methodology. CFD, pedagogy and immersive technologies are described in detail forming the main pillars of our hypothesis.

2.2 Computational fluid dynamics

2.2.1 Theory

Background

Carrying out a computational study was impractical until computers such as ENIAC were developed in the late 1940s [10]. Scientists from Los Alamos National Lab made the first known attempt using computers to solve the Navier-Stokes equations to predict the dynamic behavior of fluid flow. Over the past century, CFD has become a mainstream numerical tool intensively applied to solve engineering problems, being complementary or even an alternative to experimental methodologies. CFD requires an interdisciplinary approach

to properly set up computational studies by involving computer science, mathematics and physics. Preparation, calculation, and post-processing are a set of subsequent steps that are executed manually by a competent analyst. CFD simulation results are generally analyzed in a heavily interactive process with specialized post-processing software to obtain meaningful data in support of decision-making. Accuracy and computational time are two main parameters that analysts aim for, and often a trade-off between them exists. CFD data can come in various forms such as analytics, charts, tables, glyphs, markers, lines, 2D contours, 3D iso-surfaces and volumetric data. Not only technical and analytical skills, but also competencies such as problem-solving, critical thinking, spatial reasoning, time management and decision-making are crucial to adequately apply CFD simulations in engineering methodology.

Methodologies

Traditionally, Navier-Stokes Equations (NSE) and Lattice-Boltzmann Method (LBM) are the two main theoretical models of fluid flow based on continuum mechanics and molecular dynamics, respectively. NSE has become the mainstream theory applied in the majority of numerical solutions. Interestingly, researchers have recently shown an increasing interest in LBM due to its advantages such as efficiently structured massive parallel computational architectures, low-cost pre-processing, fully resolved multiphase flow and the ability to deal with complex geometries [46]. However, LBM is in general computationally expensive, immature in turbulence modeling and lacking industrial and academic support. Therefore, NSE is currently the most preferred theory to computationally solve multiphysics CFD problems in chemical and broader engineering [47, 48]. In this dissertation, the acronym CFD will be used to define the computational studies utilizing NSE to numerically solve fluid dynamics problems.

Real-time fluid flow simulations

There has been a rapid rise in the development of computational models to facilitate interactive real-time numerical solutions for fluid dynamics [49]. Several theoretical and numerical approaches have been revealed to accelerate CFD workflows with simplistic processing operations while incorporating both central processing units (CPU) and graphical programming units (GPU). The interactive real-time solutions are referred to as solutions where at least 24 timesteps per second are output by a numerical solver. The potential of real-time simulations has been investigated by targeting different contexts such as games [50], fire training simulation [51], chemical site evacuation scenarios [52] and fluid flow modeling [53]. Real-time simulations in design and modeling have been mostly restricted to either simpler or low-fidelity simulations. These would only seem to be helpful in teaching the basics of fluid mechanics [54]. Real-time

simulations have still mostly remained impractical to solve engineering problems. Unless results are retrieved from a database, a time gap should be taken into account by practitioners from simulations to the visualization of results.

Fluid flow simulations in games and movies

Graphics are undoubtedly the most significant aspect of video games. Various physics-based and non-physics-based techniques have been developed to obtain interactive and realistic visual effects where fluids are involved. According to Gourlay, fluid simulations in games, movies and computer graphics should comply with the following criteria: fast, controllable, detailed, flexible, scalable, plausible, beautiful, accessible, robust, interactive, parallelizable, handling multiple immiscible fluids including smoke and combustion, and providing both 2D and 3D effects [55]. In 1999, Josh Stam came up with an affirmative methodology by deriving a thoroughly simplified version of the NSE that decent computers can readily handle in real-time. It ultimately aims at providing visually realistic fluid effects such as swirling smoke past a moving character and vortex street. The methodology offers a simple numerical scheme with divergence-free calculations, meaning that calculations always forcibly converge applying arguably inaccurate and fictitious convergence criteria. Today, this methodology is still commonly utilized in computer graphics together with newly released numerical solutions to create visually accurate fluid effects for very challenging incidents such as transport phenomena and fluid-structure interaction [56]. There are certainly different needs in computer graphics than in engineering methodology. Interactive and visually accurate fluid effects are the key factors that game designers cannot compromise on. Therefore, CFD software used in engineering design and analysis are not compatible since these software fundamentally target physical accuracy that is being traded with long calculation times. Despite the advancements in computer graphics on realistic fluid effects, physical accuracy still remains drastically low and is not able to accurately handle multiphysics problems, thereby not enabling analysts to apply these tools to engineering problems. Also, the post-processing capabilities of CFD software are significantly more primitive than computer graphics.

Artificial Intelligence

Recent trends in artificial intelligence (AI) have led to a proliferation of studies where searchers are looking for ways to speed up CFD workflow while keeping accuracy as high as possible [57]. AI can help reduce pre-processing time, accelerate calculations and make credible decisions in a CFD workflow. Data-driven approaches and reduced order models (ROM) have been in the scope of CFD software developers enabling showcases for the academy and industry [58]. Nonetheless, the utilization of AI in CFD still requires expert interventions to alleviate any shortcomings that lead to inexplicable black-box models and

unreliable results. As a consequence, using intelligence systems in CFD is currently a research topic rather than a hands-on application.

2.2.2 Tools and application

Software

Several commercial and open-source CFD software have been released over the past decade summarized in the Supplementary information for Chapter 3. Ansys Fluent, COMSOL and Star-CCM+ are well-known commercial multiphysics CFD products providing dedicated methodologies to solve fluid dynamics, solid mechanics, (aero)acoustics and many others. Commercial products provide well-established customer services to support non-expert users with tutorials and learning modules. OpenFOAM has recently become a prominent open-source alternative to commercial software thanks to the support of academic and industrial communities. All these software have been utilized in engineering design and analysis, as well as in educational practices in some institutions. As far as chemical engineering is concerned; Ansys Fluent, COMSOL, OpenFOAM and Star-CCM+ are widely applied multiphysics CFD tools.

Hardware

CFD simulation software generally require a workstation to commit timely calculations. Even though personal computers can be employed in some instances, they merely provide a very limited computational capacity to perform calculations in the desired period of time and accuracy. Personal devices - such as tablets, smartphones and immersive technologies - are not yet capable of carrying out CFD simulations due to relatively low computational power. Alternatively, cloud-based service providers have been becoming popular enabling users to remotely run simulations without tackling any hardware-related issues. Companies such as SimScale provides CFD tools on web browsers where users only need an internet connection to commit CFD projects. Ansys Fluent, COMSOL, OpenFOAM and Star-CCM+ do also provide cloud premises. For example, COMSOL has a service named *Client for Android*, through which users can remotely perform CFD simulations and analyze results on a smartphone. From this perspective, cloud-based solutions are great enablers to involve portable devices in CFD workflows, instead of running CFD software on portable devices. Moreover, decentralized computational systems have recently gained much attention in the framework of digitalization and industry 4.0 [59]. In particular, ubiquitous and spatial computing are being addressed to get all electronic devices involved in a decentralized and distributed computational ecosystem, thereby increasing the functionality of portable devices in engineering [60].

2.2.3 Educational use

Traditionally, educational use of CFD simulations varies from data visualization to advanced graduate courses on numerical methods [47]. It is noteworthy that in the framework of this thesis using CFD in education primarily emphasizes CFD as an additional tool to teach methodology and case-specific engineering problems solved with CFD, not teaching a particular CFD software to students. According to Wilkes, CFD is a great enabler to increase students' intuition and cognition in both macroscale and microscale phenomena in chemical engineering [48]. The author also welcomes CFD in the classroom to make content "alive" due to the attractive visuals produced via CFD software, thereby enabling a way to get students' attention. CFD comprises not only hard skills but also comprises cognitive skills and competencies such as critical thinking, decision making, creative problem solving and time management, together with advanced spatial reasoning skills [12]. Therefore, the educational use of CFD simulations may be essential to prepare young students for real-life settings.

While engineering simulations can provide educational content to design learning experiences with easy-to-comprehend visualizations, they can also be utilized as computational tools to dynamically operate active learning environments. For instance, visualization of the mixing performance of different impellers in a stirred-tank reactor can be substantiated in an active learning environment, in which students explore CFD data to solve an engineering problem while learning the methodology of CFD in engineering design and analysis. CFD simulations, therefore, have a dynamic role to play in engineering education from two perspectives: facilitating active learning environments via a simulator and providing visual learning content. The prior often incorporates a course project to teach CFD and its methodology by using CFD software. Learning in a particular CFD solver often happens via learning by doing on 2D desktop settings. Such environments do not comprise any assistance except help options relevant to the usability of the tool. The latter is to extract and utilize accurate visual content generated by CFD simulations in order to enhance students' understanding of a particular topic in the form of multimedia such as video clips and images. However, in such practices, students cannot directly interact with simulation data, thereby merely experiencing a passive participation.

Concerning the broad applicability of CFD in engineering education – which is not only limited to advanced courses, meaningful data still can be hard-to-comprehend for novice students due to the sophisticated structure of the conventional post-processing software. Likewise, neither lecturers nor students may be acquiring relevant skills to deal with the complex nature of simulation software. CFD is generally assumed not to be user-friendly and does not provide supportive content in the context of instructional design. Engineering students

can face a high entry barrier in simulation environments developed through conventional workflows. All these can hinder the utilization of CFD simulations and simulation data in education in an effective and interactive manner.

In summary, although CFD has been a hot topic in engineering education, it has been practiced in a similar fashion for years mostly in advanced courses. Educational practices, where CFD simulations are involved, have not seen any advancements in terms of user technology, thus limiting its educational utility. CFD awaits democratization to facilitate user-friendly, accessible, interoperable and open-source environments for all stakeholders [61].

2.3 Pedagogy

2.3.1 Learning theory

Learning is a fundamental cognitive process to acquire knowledge and skills. Scientists have sought to theorize frameworks to explicate the learning process. Traditionally, learning theories describe how individuals acquire, process and retain knowledge in an activity, thereby attempting to answer the question "How does learning happen?" [62]. Behaviorism, cognitivism, constructivism and connectivism are some of the fundamental learning theories detailed as follows:

- Behaviorism: Learning happens when individuals are rewarded for the committed behaviors through a reinforced and repetitive process. Rewarding shapes individuals' behaviors. Neither self-evaluation nor self-reflection takes place, meaning that behaviors are repetitively shaped based on schemas identified by teachers [63].
- Cognitivism: Learning is a process driven by behaviors, environmental factors and most importantly internal mental processes of individuals. The received information is related to prior information to process and retain throughout mental activities. Individuals are encouraged to apply both low- and high-order cognitive skills in reasoning [63].
- Constructivism: Individuals actively partake in a learning process rather than passively received instructions. New information is interpreted by individuals to progressively construct and evolve schemas based on personal experiences and prior knowledge [63].
- Connectivism: As being relatively new compared to other theories, it conceptualizes a connected learning experience in which users actively utilize digital tools and find valuable information from their interaction with other individuals and external resources [64].

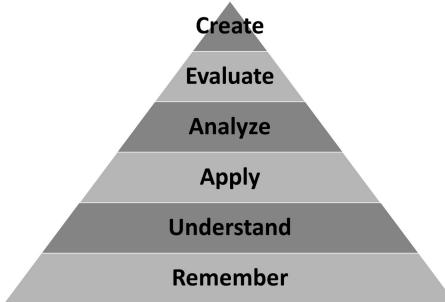


Figure 2.2: Bloom's revised taxonomy. The initial version received severe criticism due to placing the *evaluate* at the top of the taxonomy. The *create* overtook the *evaluate* in the revised version published in 2001 [67].

Details on learning theories fall outside of the scope of our thesis. Our aim is to give a foundation for methodologies we apply in the design of learning environments with immersive technology and CFD simulation.

Over the past century, learning theories have provided foundations for educational design guidelines to align learning objectives and educational practices within the needs of target groups in various contexts. A learning objective is a phrase structured by a teacher to quantify the expected knowledge and skills that a student can acquire after the course. Students' awareness of learning objectives before taking the class is vital to set their expectations and guide them through learning modules [65]. Between 1949 and 1953, researchers held a series of conferences to develop a taxonomy to help organizations determine educational objectives. In 1956, the first version of the taxonomy came out which was named after the chair of the committee of educators, Benjamin Bloom [66]. Having been criticized by researchers due to a lack of systematic rationale of construction, the taxonomy was revised in 2001 [67] and shaped to the final form that is today broadly adopted by educational organizations, as shown in Fig. 2.2. It categorizes and classifies cognitive skills to reach the utmost complexity in the learning process from low- to high-order thinking skills. The taxonomy has become a very prominent framework to effectively identify the learning outcomes in any educational practice.

2.3.2 Cognitive load and multimedia learning

Cognitive load theory

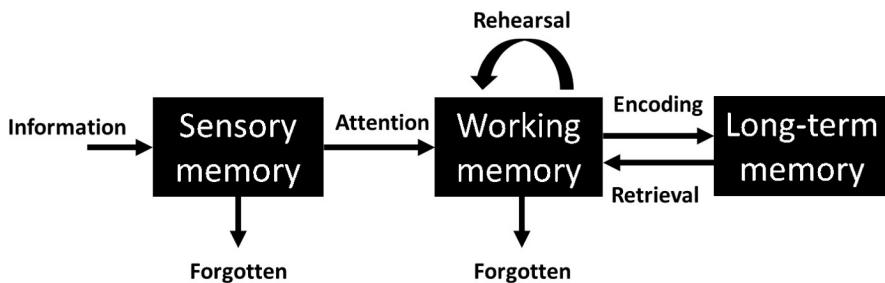


Figure 2.3: Cognitive load theory and information process model [68].

The human brain is one of the most complex systems and humankind has long been searching for an answer to understand how it processes information. Developed by Sweller in the late 1980s, the Cognitive Load Theory (CLT) has become a significant supposition explaining fundamental processes to receive, store and retrieve information in sufficiently complex content using sensory, working and long-term memories, as can be seen in Fig. 2.3 [68]. Knowledge biologically has two fundamental extents in the human brain; primary and secondary knowledge. Listening, speaking, learning and facial recognition are a part of the primary knowledge for which the human brain is biologically evolved to develop such skills. Secondary knowledge requires reasonings to process information other than primary knowledge such as domain knowledge given in schools. The CLT fundamentally explains the learning process of secondary knowledge [68].

According to the CLT, the working memory should hold the new information to enable the long-term memory to adequately process and store it [68]. The working memory has a limited capacity to process new information, and learning is impeded when it is overly laden which results in cognitive overload. The theory promotes instructional design as a tool to optimize the use of memory to prevent cognitive overload, thereby facilitating effective learning processes.

The CLT is composed of three fundamental types of loading during the learning task: intrinsic, extraneous and germane [68]. Intrinsic cognitive load defines the complexity of the information to be utilized in learning considering the knowledge of learners. Instructional design cannot manipulate intrinsic cognitive load since it is merely related to the complexity of information and the learner's prior knowledge. As an example, intrinsic cognitive load can be managed by applying the sequencing principle to sort learning content from simple to complex tasks [69]. Next, extraneous cognitive load is directly related to

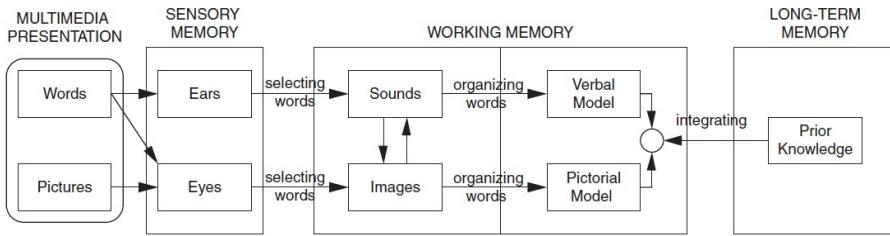


Figure 2.4: The Cognitive Theory of Multimedia Learning [70].

instructional design concerning the way of delivering instructions and actions taken by learners during the learning task. Expectedly, instructional design can deal with extraneous cognitive load. Finally, germane cognitive load refers to the process necessary to learn new information through working memory while managing resources to integrate them within existing ones. Instructional design can help control the germane cognitive load. Better learning performance results in higher germane cognitive load, whereas higher extraneous cognitive load points out a poor learning performance. To sum up, the CLT can logically elaborate on cognitive processes to effectively use cognitive load to succeed in effective learning: intrinsic cognitive load to adequately structure the learning task and align it with learners; extraneous load to prevent irrelevant and confusing information and actions; germane cognitive load to promote deep learning [68].

Multimedia learning

Recent developments in information and communication technology (ICT) have brought miscellaneous opportunities to enhance learning environments. Multimedia is the mainstream communication system to deliver information in technology-enhanced environments with words and pictures. There is a large volume of published studies describing the role of multimedia in learning [70]. Multimedia learning aims at developing cognitive representations incorporating words and pictures. In his book, Mayer proposed the Cognitive Theory of Multimedia Learning to increase the understanding of how multimedia instructions are received, processed and retrieved in the human brain as demonstrated in Fig. 2.4 [70]. Delivering instructions in the form of multimedia facilitates learning environments where individuals can profoundly learn more than only word instructions. Sensory, working and long-term memories store information with varying capacity, duration and format in the cognitive theory of multimedia learning.

The cognitive theory of multimedia learning essentially conveys five main

principles to minimize the extraneous overload when learners are exposed to multimedia instructions: redundancy principle, signaling principle, temporal contiguity, spatial contiguity and coherence principle. These five principles are evidence-based and show significantly positive effects in multimedia learning [70].

Moreover, multimedia learning theory is also widened toward simulation-based learning environments and microworlds where user actions result in dynamic responses based on a set of underlying physical models and computations [70]. Both conceptual and operational models can be implemented together with multimedia to provide an effective and efficient learning process. Physics-based computational simulation environments, in general, consist of data and knowledge represented in several forms. In a study that set out to determine the effect of linking multiple representations in a simulation environment, researchers reported that physically and dynamically linked representations showed significantly better learning experiences than the environments with unlinked representations [71]. Several other design principles to properly utilize multimedia in simulation environments are also available guiding designers to best practices [72].

2.3.3 Instructional design

Instructional design is the main pillar of the learning practices to design, develop and deliver new information through a medium that the human brain sufficiently processes. The ADDIE model is a well-known instructional design framework structuring a foundation within five generic phases to develop courses: analysis, design, development, implementation and evaluation [73]. Educational science has witnessed various principles to guide developers to create courses that can promote learning. Among many others, Merrill et al. exemplified five main principles to properly structure instructions in learning as follows; problems related to real-life examples, information and action to active existing information and relate it to new ones, demonstrations to enable observations, applications to exercise problem-solving, and integration to discuss and reflect on learned information [74].

The most prominent instructional design methodologies strongly rely on theories and models such as constructivism, cognitive load theory and multimedia learning [70]. Instructional design provides a tool to integrate new teaching and assessment methods in educational practices considering the skills of 21st century and the state of technology. Four-component instructional design, inquiry-based learning and game-based learning are well-known instructional methodologies

applied to design learning environments with immersive technologies having a basis in active learning [70].

Four-component instructional design (4C/ID)

The 4C/ID is increasingly applied in complex learning environments for the development of complex skills and professional competencies [68]. It deals with the task-centered learning environment accompanied by real-life tasks while incorporating cognitive load theory and multimedia learning. The 4C/ID model takes on a "moderate constructivist approach" regulated by guidances and supports delivered via instructions [75]. The components of the 4C/ID model are customized with several evidence-informed principles to orient tasks and instructions with specific learning objectives. A broad spectrum of principles with details is available in the relevant design guideline [72].

The 4C/ID model comprises four major components; learning task, supportive information, procedural information and part-task practice. The model facilitates schema construction and automation by utilizing memory and cognitive learning processes. While learning tasks and supportive information aim at the construction of cognitive schemas, procedural information and part-task practice give assistance to automate cognitive schemas. Learning tasks are whole-task experiences based on real-life examples in the support of schema construction. Learners are assigned to complete a set of tasks to succeed in learning objectives. Supportive information presents knowledge to educate learners about the fundamentals of the domain, methodologies for problems to be solved and cognitive examples to facilitate feedback mechanisms. Schema construction is the main target to incorporate supportive information in complex learning environments. Procedural information delivers routine aspects of learning tasks, timely guidance to correctly commit learning tasks and corrective feedback to keep users in the right direction. Schema automation is the fundamental aim to be achieved with procedural information. Part-task practice enables a drilling process to exercise repetitive procedures of a learning task where a high level of automation is crucial to succeeding in the task, as well as schema automation. Researchers point out 10 essential steps to progressively develop 4C/ID models with multimedia principles for complex learning environments to guide instructional designers [75].

Inquiry-based learning (IBL)

Minimal guidance of learners in an active learning environment does not facilitate effective and efficient learning [76]. Learners need a certain amount of guidance to find their learning path while engaging with given tasks. Unguided learning environments evidenced futile attempts in the learning process [77].

As being inherently structured upon constructivism and guided-discovery based

learning, inquiry-based learning (IBL) is an active learning environment where students actively construct meaning and solutions in the learning task. IBL aims at providing sufficient guidance based on the complexity of learning material and learners' prior knowledge. It is a process to stimulate the intellectual engagement and deep understanding of learners with real-life problems. Learners are expected to form questions, solve problems and create new solutions while collaborating with peers and lecturers. IBL activities provide the opportunity to hypothesize, explore, investigate, validate, discuss and reflect on scientific ideas [78]. IBL can foster learners' curiosity and motivation, whereas learners can gain higher-level thinking skills. Communication is an essential part of IBL through which learners are also expected to develop social and interpersonal skills.

IBL is an iterative model to be carefully designed and guided to facilitate an optimal environment for learning. *Confirmation, structure, guided* and *open* are four levels of inquiry-based learning practices, from high to low level of guidances [78]. Thanks to the advancement in educational technologies in recent years, there has been a growing interest in the design of IBL experiences in education [79]. Pedaste et al. performed a literature review to identify phases and cycles in IBL practices [78]. Upon the outcomes of the review, the authors structured a framework with five general phases in the design of IBL: orientation, conceptualization, investigation, conclusion and discussion. In another study applying the framework to develop an IBL environment to teach quantum physics in secondary schools, researchers demonstrated six instructional elements to be utilized in IBL phases: process constraints, performance dashboard, prompts, heuristics, scaffolds and direct presentation of information [80]. The IBL phases with instructional elements provide a coherent tool to develop IBL practices to align guidance and support with context and target groups.

Game-based learning (GBL)

Digital natives need to be attracted to challenges, engaging content and motivational elements in a learning environment [81]. Games are inherently constituted by these elements promoting conflicts, rules and outcomes that players seek. Competition, chance, role-playing and vertigo are the four main types of gameplay [82]. An educational game consists of a range of design elements: game mechanics, visual objects, audio, narrative, rewards, content and skills to promote a playful and motivational learning experience [83]. The Integrated Design Framework for Playful Learning proposed by Plass et al. is one of the most prominent concepts to design games that lead to a playful learning experience [84]. Cognitive, motivational, affective, and sociocultural considerations are the four main aspects of the design process incorporating game design elements.

The educational use of games has become one of the most intriguing methodologies to serve digital natives in engineering education from a constructivist point of view. Any educational experience can benefit gaming elements by logically transforming relevant components into game mechanics. Gamification, playful learning and game-based learning are three distinctive design tools to develop educational games [83]. The very first design step to introduce games in education is gamification. It essentially does not change learning activities. Instead, extrinsic rewards and narrative structure are applied throughout the learning experience to motivate learners. In contrast, playful learning is another level to design educational games by restructuring the learning task to turn it into more relevant, meaningful and interesting experiences. Instead of developing a complete game, it can promote learning experiences that partially utilize game features. In contrast, game-based learning is to design learning games using a full range of game features other than gamification and playful learning. Learning activities and instructions are accordingly reshaped to come up with more relevant, meaningful and interesting mediums. Game-based learning relies on technical content, pedagogy and gaming to properly structure learning activities. Moreover, Plass et al. categorized educational games concerning functionalities regarding overall goals and relatedness to learning [83]: preparing for future learning, acquiring new knowledge and skills, practicing existing knowledge or skills, and developing learning and innovation skills.

Educational games have long been in the scope of researchers to diversify learning tools using various technologies from mobile games to virtual reality [85]. More recent attention has focused on the evaluations of digital learning experiences and student assessments to validate design guidelines and provide evidence of their utility, respectively [83]. Remarkably, Plass et al. argue that it is vital to optimize and validate design aspects of an educational game via usability, design-based and value-added research before focusing on cognitive, affective, motivational, and sociocultural aspects [83]. Likewise, media comparison research can be also conducted to give credible arguments and evidence for policy-makers and all administrative stakeholders of an educational ecosystem in the support of the adoption of educational games.

2.3.4 Immersive learning

Immersion is a term to describe the state of being entirely absorbed in an activity, experience and environment, according to the Britannica Dictionary [86]. The meaning of immersion can significantly vary among disciplines. In physics, immersion refers to the act of being completely engulfed in a liquid, whereas it is used to describe complete mental involvement in an activity or

experience in psychology. For example, a reader can get immersed in a book with a human-centric narrative by being actively involved in the story rather than an observer [87]. Similarly, users in a VR experience can feel the sense of being immersed in a virtual environment, typically achieved through the use of specialized technologies and hands-on activities to provide sensory input that simulates a real-world environment. Immersion can refer to several other states from language education to religion to business.

Immersive learning is increasingly recognized in various disciplines to promote the feeling of being active and present that can positively affect cognitive, affective and behavioral domains. Despite the recent growth in immersive learning research, there is ongoing ambiguity over the definition of immersive learning. Dengel described immersive learning as an "artificial experience perceived as non-mediated" that evolved toward constructivism [88]. Literature has often addressed immersive technologies as the main driver of immersive learning [89]. Some attempts have been made to highlight the significance of both design and cognitive aspects over technological ones to manifest an immersive learning framework [90]. A recent study suggested that immersive learning is intrinsically focused on the impact of immersion on the learning and perceptual processes regardless of any technological interference [88]. A framework to involve technology in education such as SAMR can facilitate a tailor-made process to design and develop digital artifacts for immersive learning environments with technology [89].

In the context of immersive technologies, immersion can precede the presence [91], interaction and imagination [92] in varying degrees. The feeling of being actually and physically present in a fictitious or distanced environment is referred to as presence [93]. The presence can be governed by sensory stimuli driven via the level of immersion and functionalities of immersive hardware [94]. Likewise, interaction describes the aspects of associations between humans and computers [95], which is relevant to the level and fidelity of the control that is given to a user. Immersive experiences can exploit interaction in miscellaneous interferences by implementing complementary hardware such as head-mounted displays, sensors and hand controllers. In addition, imagination is defined as a significant attribute of VR experiences controlled by the content of the virtual environment, which can promote a high level of involvement [96].

Immersive technologies have a role to play in immersive learning to enhance immersion, presence and interaction throughout a direct physical intervention and sensor stimuli [97]. Immersive learning with immersive technologies can offer supplementary or complementary tools to overcome the limits of traditional learning practices. It can provide the possibility to visualize abstract concepts or unobservable scientific phenomena in a safer and more accessible manner with cheaper and scalable solutions. It is noteworthy that technology is an

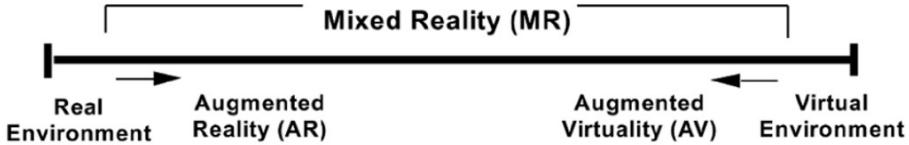


Figure 2.5: Reality-virtuality continuum by Milgram [98].

enabler for enrichment in the immersive learning environment. The learning experience should be rather designed by applying suitable instructional design guidelines as a key component of the pedagogic effectiveness in learning practices. Dengel claimed that there is an intriguing interplay between immersive learning, multimedia learning and game-based learning [88]. Lack of instructional design has existed as a major problem in the adoption of immersive learning experiences with immersive technologies in engineering education [88, 89].

2.4 Immersive technologies

2.4.1 Augmented and virtual reality

Conceptual framework and background

In 1993, Milgram conceptualized the reality–virtuality continuum to define the degree of virtuality between real and virtual environments, including augmented reality (AR) and mixed reality (MR) in between [98], as can be seen in Fig. 2.5. Even though the continuum does not sufficiently represent the current state of the entire immersive technology spectrum, it depicts an abstract level to conceptualize and differentiate the level of immersion for beginners.

Virtual reality (VR) is a digital environment in which users are cognitively immersed through sensory stimuli in a fully digital space. The first hands-on VR experience dates back to the 1950s when Morton Heiling unleashed "the Sensorama concept" as illustrated in Fig. 2.6 [99]. He aimed to prototype a VR experience combining video, sound, fans and vibrations to trigger the sensory stimuli of riding a motorcycle. However, the prototype did not receive enough financial support and was therefore not commercialized.

Augmented reality (AR) refers to an enhanced digital experience where digital assets are superimposed on real objects. Simultaneous interaction with digital assets and real objects from a digital experience is termed mixed reality (MR).

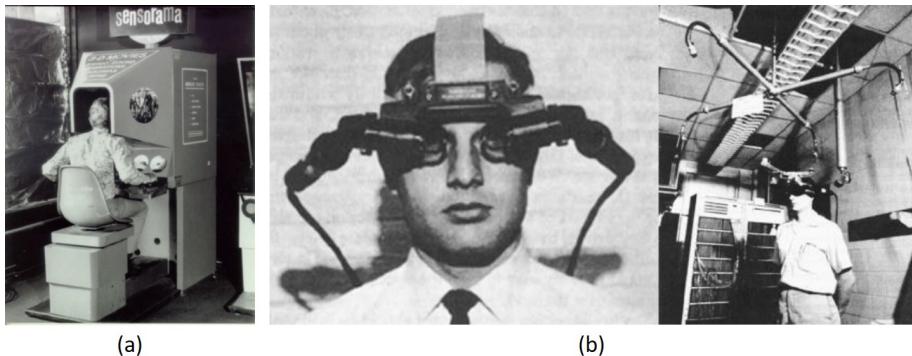


Figure 2.6: The Sensorama concept as a forerunner of VR prototypes [99] (a); the ultimate display as the first known AR prototype [100] (b).

The first known head-mounted AR device was "the ultimate display" developed by Harvard professor Ivan Sutherland and his student Bob Sproull in 1986 [100]. The device was so large and heavy that it was suspended from the ceiling directly above the user as shown in Fig 2.6. It had some basic features such as head-tracking. It was not until 1990 that a major breakthrough in AR was revealed by Tom Caudell, a researcher at Boeing and forefather of the term augmented reality. He was seeking an alternative training to traditional instructions for workers who were installing the wirings on planes. Caudell and his fellow colleagues conceptualized a head-mounted AR prototype superimposing the wiring connections onto a board, thereby interactively guiding workers during on-site manual assembly.

Today, AR and VR have become publicly accessible technologies demonstrating miscellaneous real-life applications and showcases from entertainment to education. Notably, engineering education has shown an increased interest in immersive technologies to digitalize and diversify educational tools to open gates for accessible, inclusive and high-tech educational practices [101, 20].

Immersive hardware

For many years immersive devices have been labeled as future and emerging technologies due to the potential enhancement they could bring to everyday tasks. Until recent years, VR hardware has been operated via bulky headsets, powerful computers and custom peripheral devices, resulting in expensive, non-ergonomic and complex systems. Similarly, AR hardware has long only been developed as proofs-of-concept hindering enthusiasts to access technology because of the high prices and the low market readiness. Hence, the wide adoption of

immersive hardware has not materialized for a long time. Rapid advancements in smartphones, however, have now become the driving force behind immersive technologies to develop advanced AR and VR devices equipped with various sensors to unleash their full potential. Fig. 2.7 demonstrates examples of recently released immersive hardware commercially available.

A modern version of VR hardware is composed of a headset and hand controllers to enable a fully immersive digital experience. These hardware are equipped with sensors, tracking devices and cameras to stimulate immersion, interaction and presence in VR environments. Not only technical specifications but also ergonomics play a crucial role in the adoption of VR devices by individuals to improve the quality of the VR experience. Nowadays, both standalone and PC-connected VR hardware is available in the market providing a diverse range of computational power at affordable prices. The better VR devices get, the better VR experiences are inherently developed. Recent surveys prove that hardware is the key enabler in the research, implementation and adoption of immersive technologies [102]. The VR hardware market has a dynamic trait of incrementally improving hardware quality, affordably and accessibility. It is not unlikely that a new VR device will drop into the market to enable a function that we were not capable of while this thesis was being written.

As opposed to its VR counterpart, AR has a diverse hardware spectrum to operate immersive environments. AR hardware can be classified into two main categories: Video-See-Through (VST) and Optical-See-Through (OST). VST devices such as smartphones and tablets are decently equipped with sensors, tracking devices and cameras that are required to run AR software. Similarly, recently developed VR headsets such as Meta Quest 2 feature a VST option enabling both head-mounted display (HMD) AR and VR experiences within the same device. The VST AR relies on a camera to capture the real environment and superimposes digital objects into video streaming. VST-based AR experiences enable cheaper and simpler solutions to augment real-life experiences with digital additions. In contrast to VST in which the user sees the real environment from a screen or display, OST devices such as Microsoft HoloLens projects digital object onto semi-transparent glasses through which the user directly sees the real world. OST devices are in general composed of more powerful and complex hardware to additionally support MR software, thereby costing a lot more than VST.

Beyond the capabilities of mainstream commercial hardware, developers have also concentrated on auxiliary equipment to leverage immersive technologies for case-specific applications, integrating external custom haptics and wearables. The main aim is to amplify the level of immersion through auxiliary hardware synchronized with immersive technologies such as gloves to feel temperature, gadgets to smell scents and custom tools to control simulation environments. In



Figure 2.7: Meta Quest 2 VR HMD headsets [103] (a); Microsoft HoloLens MR glasses [104] (b).

particular, a few studies have focused on the development of haptics to increase users' interaction with engineering simulations such as committing geometric manipulations and volumetric data exploration [105, 106]. Recently developed immersive hardware can enable almost identical functionalities via graphic user interfaces and hand controllers as default.

Immersive software

Previously, developers needed to figure out a vague workflow to develop AR/VR applications implementing compatible plugins with their devices and design tools. In the past years, poorly structured workflows resulted in an unmaintainable immersive software ecosystem [107]. Recently, game engines are providing exclusive frameworks and platforms to create a sustainable immersive software development ecosystem to achieve long-lasting and maintainable immersive experiences. Expectedly, the utilization of game engines in immersive software developments has skyrocketed to create custom AR/VR software that can be deployed on mainstream devices. Notably, Unity and Unreal Engines are the mostly utilized game engines to deploy cross-platform applications from computer games to VR. They facilitate a user-friendly software development ecosystem continuously integrating software development kits (SDK), application programming interfaces (API), plug-ins and custom tools to meet the industrial standards and demands of immersive technology developers. Both commercial and open-source workflows can be pursued to obtain the desired immersive environment from AR to VR with custom design features. There are open-source plugins such as OpenXR bundling a wide range of provider plugins under one environment comprising both AR and VR.

Oculus XR, SteamVR, Windows MR, Google VR and Samsung Gear VR are

plugins to create specific VR experiences in different hardware. VR experiences can vary based on the employed device. Traditionally, sensors and tracking features available in VR headsets define the degree of freedom (DoF) from 3 to 6, meaning the number of movements that users can commit. 3 DoF merely lets rotational motion in which the user is statically positioned in a VR environment, whereas 6 DoF additionally enables translational motion. Head tracking, hand controllers, hand tracking and gaze tracking are commonly substantiated features to let users move in VR environments.

Furthermore, Google ARCore, Apple ARKit, PTC Vuforia, Windows XR and Magic Leap XR are plugins to enable the development of AR software via game engines for various devices. The common AR methods reported in the literature are marker-based, markerless-based, and location-based tracking. Overall these techniques involve tracking the user's position and orientation by means of sensors available in the device to position the virtual objects relative to the real environment. Marker-based tracking uses computer vision technology that allows comparison against an image or database of images, after which 3D virtual objects can be positioned in real-time. If only objects naturally present in the scene are used to determine the position, the method is called markerless. Location-based AR uses the sensors from the device and the positional data determined by the Global Positioning System (GPS) to superimpose the virtual content.

Moreover, multimedia and 3D modeling are significant assets in the design and development of immersive environments. Various open-source and paid assets can be readily obtained from the assets stores of Unity and Unreal Engine. Communities have been growingly sharing assets adapted to immersive environments reducing the need for technical skills in 3D modeling. In some instances, developers can also build and design 3D models via 3D computer graphics software such as Blender, Maya and 3ds Max, as well as computer-aided design (CAD) software. 3D modeling in engineering software such as CAD is based on Non-Uniform Rational B-Splines (NURBS), which comprise mathematical representations of 3D geometry. It can create geometry models with a high degree of accuracy consisting of 2D lines, curves and splines, thereby requiring a certain amount of computational power. In contrast, game engines adopt polygon modeling which always calculates straight lines between points, rather than creating curves and splines. Although 3D models created with polygon modeling can result in more abstract features, it comes with a computational advantage requiring less power than NURBS. Therefore, in general, there is a need for a data processing pipeline to transform CAD-based 3D models into suitable data formats to import into game engines. Meanwhile, any other external multimedia tools such as images and videos can be directly imported into game engines as long as complying with supported data formats.

Aside from technical development workflows, literature has witnessed a huge growth in the human-centric design of immersive environments [108]. Human factors concerning both physical and psychological aspects should be carefully taken into account concerning target users, context and content of the immersive experience. Governing bodies such as European Union (EU) [109] and standard organizations such as the International Organization for Standardization (ISO) [110] are continuously providing and improving policies and guidelines in light of the latest shreds of evidence to create better user environments with immersive technologies.

2.4.2 CFD data in game engines

Multiphysics CFD simulations are powerful computational tools to create high-quality, accurate and visual engineering content. In particular, the extraction of the simulation dataset is an important stage to deal with large simulation datasets, according to the NASA CFD Vision 2030 [111]. Visualization, management and integration of simulation data should be better developed in simulation software to enable engineers to carry out a complete simulation project within a restricted time and make decisions. Automation of the CFD workflow, database management, validation, visual representation, real-time processing, multiphysics simulations, multiplatform processing and novel visualization methods of simulations (AR/VR) are identified as the key areas for further improvement in this realm.

The integration of CFD results with game engines has recently received scholarly attention to benefit educational content in AR/VR following two main approaches: reprocessing text-based CFD data directly in game engines [112], and processing and importing visual data extracts into game engines [113]. Several studies have also proposed the update of CFD results in the AR/VR environment by using dedicated remote and cloud servers [35, 32]. Another study reviewed engineering simulations in AR from a systemic perspective [16]. The study concluded that the integration of CFD data with AR/VR is mostly done with very unique elements using specific software, hardware, and dataflow pipelines. Literature is still missing an inclusive system architecture to guide practitioners. In addition, researchers have mostly reported platform-specific, computationally demanding, non-replicable and manual integration methodologies [16, 17, 114]. Digital applications are generally hardcoded, platform-specific and standalone, comprising a static CFD post-processing without any connection to a CFD solver or data processor. Technical integration of simulation data with cross-platform software should still be studied to obtain long-lasting digital applications concerning software development workflow, remote connection, data visualization, and user assessment. A conclusion has

still not been made on how to post-process big CFD data into manageable parts, which an AR/VR development platform and user's device can handle. Challenges on the hardware and software sides are still persistent in the integration of CFD data in game engines.

2.4.3 Immersive learning with CFD

Immersive learning environments may reduce the entry barrier to cognitively complex learning subjects in a safe, cheaper and scalable way [15]. They can positively trigger higher cognitive skills and advanced spatial interactions with visual, interactive and easy-to-access technical content [115]. Notably, immersive technologies provide the possibility to visualize abstract concepts or unobservable scientific phenomena, such as magnetic fields and fluid dynamics [116]. Visualization of CFD data in VR can enable a better interface than 2D screens to work with complex datasets in the context of scientific visualization [38].

AR/VR can provide a new medium for educational practices with CFD simulations by facilitating immersive and interactive user experiences. Many researchers have investigated the integration and implementation of CFD simulation data in immersive technologies, particularly for visualization purposes [112, 16, 114]. According to the initial evaluations, the immersive tool seems beneficial to improve the understanding of students on content but still misses significant elements in the design of the educational experience [29, 105, 117, 118, 119]. Given the complexity of CFD workflow and methodology, immersive visualization of CFD simulations in AR/VR is not sufficient for non-expert users. The learning environment should be adequately structured considering relevant components of pedagogy and instructional design.

User applications are still lacking technical and pedagogical design elements. No attempt has yet not been made to design, develop and evaluate an immersive virtual reality learning environment with CFD simulations. Interestingly, a number of researchers have addressed that more research on the evaluation of digital products and user assessments including human factors is essential to provide better applications and unlock the potential of these tools from students to policymakers [16, 17, 39, 114].

2.5 Conclusion

In this chapter, the current state of knowledge was presented about how immersive technologies can be applied in support of engineering education with CFD simulations. Fundamentals of CFD, pedagogy and immersive technologies were given to set a basis for our work. In the first part of the state-of-the-art, we described CFD simulations and their educational use concerning available challenges to increase learning efficiency. In the second section, we expanded our knowledge in pedagogy to answer the questions "how does learning happen?" and "how to design a learning experience based on context and content?". In the final part, we presented immersive technologies and their integration with CFD simulations. The state-of-the-art guides readers to understand and interpret the interdisciplinary research presented in the following chapters.

Chapter 3

Automated integration of extract-based CFD results with AR/VR in engineering education for practitioners

Based on a published manuscript: *Solmaz, S., & Van Gerven, T. (2021). Automated integration of extract-based CFD results with AR/VR in engineering education for practitioners. Multimedia Tools and Applications, 81(11), 14869-14891. <https://doi.org/10.1007/s11042-021-10621-9>*

Author contributions: S. Solmaz conceived the research, performed the data analysis, interpreted the results and wrote the article. T. Van Gerven contributed with his guidance and expertise in this work.

Abstract Computational fluid dynamics (CFD) simulations can provide meaningful technical content in engineering education, broad engineering and business. However, computationally demanding data production and complex data processing environments of CFD simulations turn them into esoteric tools for potential non-expert users. This consequently limits applications and communications of CFD simulations and results. Augmented and virtual reality (AR/VR) technologies are opening new gates for visualization and interaction techniques. Despite the many recent attempts, the literature lacks an inclusive system development procedure for CFD simulations with AR/VR. The present study proposes a component-oriented system architecture to generate dedicated

workflows for any kind of AR/VR environment supported by CFD simulations. The study further explores the potential of data processing options throughout the preparation of the simulation dataset with AR/VR. An automated data coupling strategy is additionally introduced to ease multiplatform integration. We provide an integration strategy with simple, easy-to-implement, end-to-end, automated and free-to-use utilities that the practitioners can readily pursue.

3.1 Introduction

Computational Fluid Dynamics (CFD) simulation tools are powerful alternatives to experimental campaigns because of their cost- and time-effectivity. Visualization, virtual experiments, and prototyping are profound features of CFD simulations. Preparation, calculation, and post-processing are a set of subsequent steps that are executed manually by a competent analyst. CFD simulation results are generally analyzed in a heavily interactive process with specialized post-processing software to obtain meaningful data in support of modeling and design. However, meaningful data still can be hard-to-comprehend for inexperienced users (e.g. engineering students) due to the sophisticated structure of the conventional post-processing environments [17].

Decision-making in engineering is getting challenging because of the increasing complexity of technical subjects. Augmented and virtual reality (AR/VR) can help communities to deliver more visual and interactive digital products through a better understanding of physical phenomena with meaningful, realistic, easy-to-comprehend, functional and attractive digital environments [120, 16, 41]. This can reduce the communication gap between CFD simulations and broader engineering including students, clients, customers and stakeholders. CFD simulations may even be utilized to operate active learning environments in engineering education (e.g. inquiry-based learning, game-based learning and learning-by-doing) due to their computational nature. Nonetheless, the lack of desired digital content and content integration methodologies are the missing building blocks in the development of digital applications [121, 16, 23, 17, 40].

The integration of CFD results with AR/VR recently received scholarly attention. Literature has still been missing an inclusive system architecture to guide the practitioners [16]. The term system architecture is used as a portrayal of the system that consists of software and hardware including their functionalities and interactions [122]. Besides, platform-specific, computationally-demanding, non-replicable and manual integration methodologies have mostly been reported by researchers [16, 17]. A conclusion has still not been made on how to post-process big CFD data into manageable parts, which an AR/VR development platform

and user's device can handle. Additionally, no study has been reported on the multiplatform integrity to assess the data processing performance through data format, size, processing time, quality, automation and management. These ambiguities prevent practitioners to utilize AR/VR tools to visualize simulation data [16, 17].

3.1.1 Contributions

The objective of the present research is to provide a technical development strategy in support of practitioners to use CFD simulations with AR/VR in engineering education. Our research discloses significant contributions:

A system architecture to develop educational tools with CFD simulations and AR/VR. It proposes an inclusive guideline on the multiplatform integration targeting miscellaneous workflows and excellence of each utility with component-oriented structure.

A robust approach to adapt CFD data with AR/VR. We provide an extract-based data processing approach to integrate any type of CFD visual representations. Methodologies provide alternative features upon simple, easy-to-implement, end-to-end and free-to-use utilities.

A qualitative assessment on multiplatform integration. Multiplatform integrity is examined based on data format, size, processing time and quality. This is significant to elaborate extract-based data processing methodologies and determine suitable utilities.

An automated one-way data processing pipeline. A Python script enables a soft-coded, modular and automated end-to-end integration of CFD datasets in the game engine.

A descriptive guidance on the management of data in use. We provided a comparison among data models to store and retrieve CFD datasets in manageable parts throughout the integration.

The findings of the present study will help practitioners to integrate desired simulation results with the aid of newly adapted technologies in engineering education.

3.2 Related work

3.2.1 Expectations in CFD simulations: experts vs. non-experts

A CFD simulation can be used in many contexts such as engineering design and optimization projects, training and educational materials, and video games. It is conjectured on a cost function that is composed of certain parameters to tune from geometry to representation of results. Accuracy and frame rate (or run-time) are the most significant outputs revealed from the cost function. The accuracy points out the difference between the obtained and standard values. The frame rate refers to the total number of datasets produced per second. Depending on the context of the simulation, the accuracy and frame rate are modified to develop the desired simulation content. While a video game requires visually credible assets with relatively high frame rates, engineering simulations rely on physics-based models with high numerical accuracies.

Literature claims a continuum between accuracy and frame rate for CFD simulations [123], without, however, quantifying thresholds for these two criteria. Fig. 3.1 demonstrates a widened continuum to detail the current state of CFD simulations. Firstly, physics-based and fluid-like modeling approaches are the two distinctive methodologies to set a clear boundary between the levels of accuracy. Secondly, the frame rate of a simulation can be defined either batch or real-time. Compared to batch, real-time simulations should solve and process at least 24 frames per second (fps) [124]. The potential of real-time CFD simulations has been investigated targeting different contexts such as games [50, 125], fire simulation [126], chemical site evacuation scenarios [127] and fluid flow modeling [128]. Although, real-time simulations in design and modeling are still in their infancy, thus mostly impractical to use in multiphysics CFD modeling. Unless results are retrieved from a database, a time gap should inherently be taken into account by practitioners from simulations to the visualization of results.

3.2.2 Integration of CFD simulation data with AR/VR

The extraction of the simulation dataset is an important stage in CFD simulations, according to the NASA CFD Vision 2030. Visualization, management and integration of simulation data should be better developed in simulation software to enable engineers to carry out a complete simulation project within a restricted time and make decisions. Automation of the procedure, database management, validation, visual representation, real-time processing,

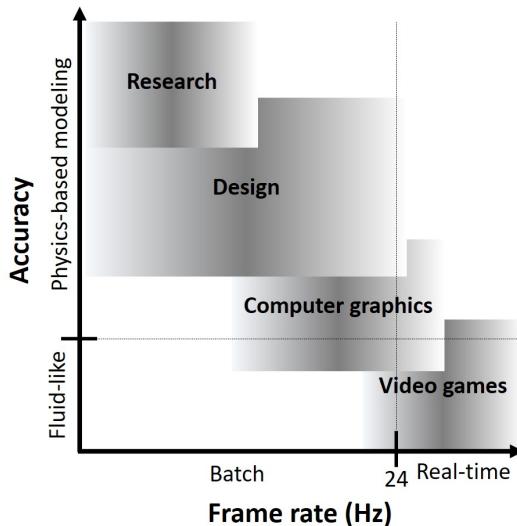


Figure 3.1: The continuum of CFD simulations concerning accuracy, frame rate and context.

multiphysics simulations, multiplatform processing, novel visualization methods of simulations (AR/VR) are identified as the key areas for further improvement in this realm [111].

In the literature, various approaches have been proposed on the system development to integrate CFD simulation with AR/VR. Likewise, a variety of data processing methodologies have been suggested to structure digital resources. The following sections review available development approaches and data processing methodologies.

System development: hardware and computational challenges

He et al. proposed an integration methodology on CFD simulations with AR/VR via cloud computing [31]. The main disadvantage of the methodology is that only support of cloud computing is considered whereas other network possibilities were dismissed. Similarly, Kim et al. proposed a framework built upon the CFD simulation, AR post-processing, and AR visualization together with devices and cloud servers [32]. Although both studies explain well the system components, the procedures and requirements to develop the system were

excluded. Another shortcoming is that the focus on specific AR/VR features provides a restricted system architecture to replicate the methodologies.

Cha et al. designed a system architecture for fire training simulators including four main components: training and evaluation logic, hardware and software resources, human-computer interaction, and end-user simulator [51]. A system development procedure was promoted with user-specific components and dataflow. Another system architecture was detailed by Yu et al. including dataflow and system requirements but thoroughly structured with dedicated system components too [129]. Software, hardware, and network options were defined as fundamental system elements to develop digital environments.

System development procedures for real-time simulations were recently reported as well. Harwood and Revell compared dataflow methodologies of interactive simulation to those of traditional simulation [53]. Even though procedures to run every single component can vary, both simulation techniques are designed on similar system elements.

Researchers showed interest in the Internet of Things (IoT) to interact with the physical environment. An approach was demonstrated to process energy performance data with augmented reality in buildings [30]. Another study evaluated the design phases of a system to use sensor data with AR/VR [130]. The studies revealed that IoT devices can leverage the interaction with simulation results through the real-time measured data from the physical environment.

Only a few studies have shown direct interest in database and management systems of simulation datasets in system architecture [131, 132]. The CFD Vision 2030 report from NASA states that real-time querying of large databases and continuous update of these will be quintessential in the near future [61]. A database management system is a must to save, store, reproduce, and reprocess simulation datasets.

To sum up, system development procedures were principally structured on software, hardware, dataflow, network, IoT, and database to design digital environments. Researchers' interest in task dedicated subjects to integrate simulation datasets resulted in very specific system development procedures. A generic system architecture to guide the practitioners is not available yet.

Data processing: software and data handling challenges

A CFD dataset is usually stored in a data exchange format pertinent to the CFD solver. It can be either a dedicated or text file format that is commonly used for the storage of information. Both can only be processed with CFD post-processors, not with any other 3D computer graphics software without

required post-processing algorithms. Therefore, a data processing methodology is required to adapt CFD data with AR/VR development platforms such as game engines. In contrast, supporting multimedia (image and video) and analytic data (direct or derived results in text format) exported from the post-processor can be directly imported into game engines without any further manipulation. Both CFD post-processors and game engines give support for the most common multimedia types and data formats.

Visualization of CFD data can be categorized as vector-, surface-, and volume-based. In recent years several 3D data formats have been released to encode digital visual objects. A 3D data format mainly consists of information on geometry, texture, scene and animation. Researchers have investigated the applicability of different 3D data formats to integrate the CFD simulation dataset with AR/VR. STL [133] [134], 3DS [35], VRML [135, 136, 137, 113], FBX [135, 138, 113], DAE [139], and X3D [133] were commonly applied with several CFD solvers, post-processors, and 3D computer graphics software to achieve the integration. It is observed that complex structure of CFD dataset and arbitrary nature of data processing make a comparison among studies almost impractical.

Processing of a CFD dataset with the Visualization Toolkit (VTK) is popular among researchers. Huang et al. developed an interactive AR-based finite element method (FEM) simulation environment with VTK [140]. In another study, Kim et al. processed a CFD dataset with ParaView and VTK to develop an AR application [32]. Wheeler et al. structured a plugin to export VTK data format to Unity [141]. These studies fundamentally reported user-defined data processing methodologies to import VTK files into Unity. Lin et al. additionally developed a data format to reduce the data size and loading time of CFD dataset against VTK format in a mobile device-based AR [117]. The main weakness in many of these studies is that they overlook the processing of datasets produced by any other CFD solver that cannot be turned into VTK format without a wrapper [142]. Such a processing method restricts the applicability of other CFD software. In addition, game engines do not support VTK format so that practitioners may rely on unofficial data processing pipelines. This can adversely affect data size, processing time and, more importantly, quality and replicability.

Visualization of simulation datasets with AR/VR embedded post-processors [143, 144, 145] and web-based post-processing environments [146, 147] were also found nascent applications. Yet, both approaches are designed on intricate post-processing environments of engineering software which restricts data exploration and user interaction significantly [17].

Contrary to 3D data formats, test-based data extractions (such as CSV and TXT) can be utilized to integrate CFD dataset with AR/VR. Berger et al. were

among the first ones who developed a plausible workflow for a simulation dataset to create 3D visualization directly in the game engine [112]. Yao et al. [148] and Kim et al. [149] also reported similar user-defined and manual processing methodologies. These studies suffered from many pitfalls. Initially, the relevant CFD data post-processing algorithms should be reinterpreted and recompiled in the game engine to reproduce CFD visualizations from a text file. While this method may be computationally demanding for large datasets, it would also require compatible hardware to execute the data processing. This results in an enormous amount of redundant work that can readily be handled by CFD post-processor and 3D data extracts. The methodology is also generally applicable for streamlines and similar structures, not any other visual representations to explore multiphysics CFD simulations (contours, iso-surfaces, and iso-volumes). Besides, switching to another game engine can undermine the effort put in the former platform because of differences in application programming interfaces (API). Nevertheless, reprocessing the CFD dataset in a game engine would be beneficial if an interaction is required in the end-user console to manipulate the CFD results for some reason.

Representation of analytic data can be handled in several ways. Graphs are often reproduced with CFD post-processors to interpret results. Exporting a graph in image data format enables the direct import of digital assets to a game engine without any further manipulation of the dataset. A CFD dataset can alternatively be reprocessed with 3D computer graphics software to generate interactive 3D graphs in AR/VR. Using game engines for scientific computing and data analytics extends their applicability to represent analytic results [150]. Several open-source plugins have been reported in the literature enabling direct reprocessing of TXT and CSV for visual interactive analytics [151, 152].

3.3 Methodology

In an attempt to develop generic system architecture, we propose an extended methodology on the integration of CFD simulations with AR/VR. Not only CFD simulation but also a well-structured dataset from an experimental study can be implemented in the present methodology. The prior aim of the system architecture is to present a scaffold for a multiplatform-based generic system development procedure targeting miscellaneous workflows. This allows practitioners to integrate simulations with AR/VR and orchestrate a system within its components.

The system essentially deals with multiple platforms through unique operations. We pursue a component-oriented development strategy to handle the diversity

of software in the integration of CFD with AR/VR. A sustainable integration can solely be achieved considering the excellence of each component. A similar approach for a software development procedure was detailed to avoid monolithic entities as well as to reduce the development cost by utilizing components already available [153].

3.3.1 Generic system architecture

A system is composed of components, requirements, hierarchies, and other fundamental elements depending on the discipline it is used for [154]. In the present study, a system architecture directly targets a canvas that is made of software, hardware, functionalities, and connections between each system element.

A system architecture is proposed in Fig. 3.2. At first, *components* are defined to express main tasks to achieve multiplatform integrity. Each component encompasses *sub-components* in which a part of a task can be executed subsequently. Secondly, *system requirements* are proposed to convene specifications for each component and sub-component where required. Operating system, software, hardware, add-in, network, programming language (application programming interface, compiler or interpreter), and IoT are classified under the system requirements. They are determined based on their added values as reviewed in the literature. System requirements offer a toolbox of functionalities to execute dedicated tasks in the development. The final element of the system architecture is the *dataflow* that indicates the procedural interaction between system components.

User experience may indirectly contribute to the system architecture. Molonet et al. illustrated a system to evaluate user's interaction with simulations inside a game engine together with learning analytics [155]. The primary focus was on how the end-user environment affects the system architecture and development. Besides, dataflow additionally comprises possible design strategies that can be applied upon pedagogical concerns [156]. Hamilton et al. reviewed an approach to design learning environments with relevant academic content and technological support [45]. The study claimed the significance of users' interferences in the development and design of learning environments. These aspects are included in the system architecture within the form of *indirect components*.

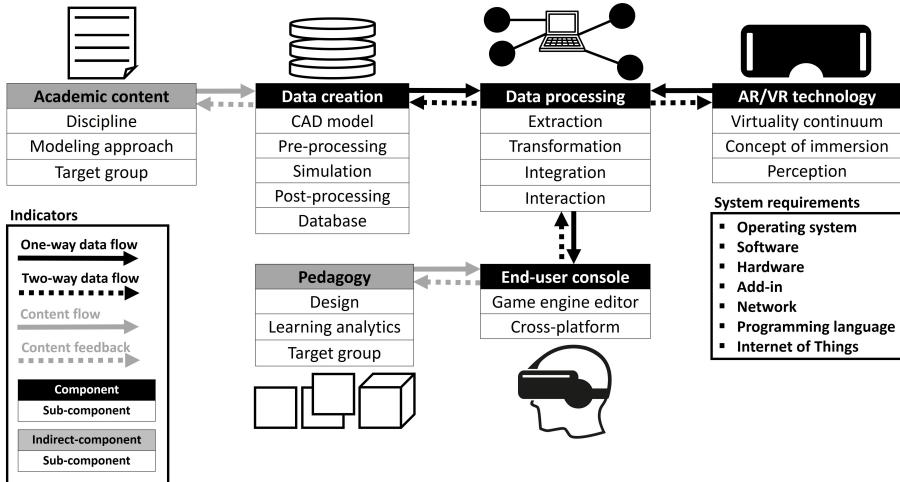


Figure 3.2: Generic system architecture to integrate CFD simulations with AR/VR.

3.3.2 Visual representations of simulation datasets

A CFD solver produces simulation results in a native data format which points out specifically encoded analytic results. These results generally consist of large, complex, and transient datasets of solutions of partial differential equations. In that sense creating data extracts from native CFD data can contract data size drastically [132]. Results in native format can also be processed and exchanged to interoperable CFD data models during the extraction for multiplatform usage. Moreover, processing of a simulation dataset to generate meaningful visual representation requires technical expertise. Thus an analyst should optimize the CFD post-processing workflow in advance for inexperienced users.

Visual representation of CFD results can be compartmentalized as vector-, surface-, and volume-based. Vector-based visualization consists of a vector field within point and gyroids. It provides a very restricted visualization to interpret simulation results. Surface-based visualization enables layers with dedicated textures to visualize results. Likewise, volume-based representation, for instance, streamlines, is the most visual type of data representation due to the inclusion of 3D geometry and texture together. To export the visual representation of a CFD dataset, a post-processor or 3D computer graphics software should be employed to produce extracts in 3D data formats. Fig. 3.3 presents extract-based data processing methodologies to integrate CFD data with AR/VR. The

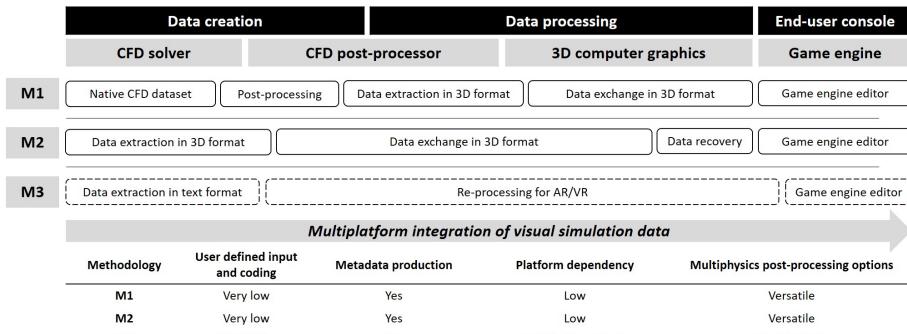


Figure 3.3: Components implemented in the methodologies are shown with solid outlines. Components with dashed outlines (only appearing in M3) mean that no implementation has taken place in the present work.

integration may comprise several intermediate data formats and software due to the interferences of multiple platforms. Methodologies M1 and M2 were thoroughly assessed in the present study due to the advantages brought in the data processing. M3 was neglected in the present study due to platform- and simulation-specific, computationally demanding, and time-consuming features.

3D data formats, to generate 3D digital visual contents, comprise a geometry and can also be composed of texture, scene, and animation. Hence, visual representations of CFD datasets are alike to any 3D data exchange formats used in 3D computer graphics software as proposed with methodology M1 and M2. More details on 3D data formats (developer, license, data type, and data encoding characteristics) can be found in the Supplementary information for Chapter 3.

3.3.3 Database and management system

A CFD solver operates large and complex simulation datasets. A database and data management system might be required to access (save, store, search, trace, and compartmentalize) and process (import, export, reproduce, and reprocess) data, and prevent any data loss or falsified action. Database management systems (DBMS) are platforms to organize data and databases to avoid the drawback of a traditional file-based system. A DBMS prevents data redundancy and inconsistency, difficulty in accessing data, data isolation, insecurity, transaction problems, non-traceability, and several other downsides of file-based systems [157]. Commercial and open-source CFD software provide

well-designed DBMSs. No further action is needed to manage simulation datasets except for the necessary hardware as physical storage. Nevertheless, the integration of CFD with AR/VR unleashes a multiplatform data processing procedure. The data can be encoded with a 3D data exchange format that is unfamiliar to the CFD simulation software. Thus, an additional database system can be implemented to manage intermittent and unfamiliar metadata formats. Beyond, a database system for CFD with AR/VR may enable the practitioners to integrate many outsource data from CFD databases developed by scientific communities, application galleries of CFD software, and even academic publications.

3.4 System implementation

A case study was performed to assess the system architecture. We widened the case study to investigate the current data processing methodologies through data formats and software. Beforehand, exploratory work was carried out to review applicable data formats (see the Supplementary information for Chapter 3 for details). As a benchmark, a CFD study for the 3D transient mixing process in a stirred tank was performed to sample CFD data. It was processed to develop a mobile marker-based AR application. A workflow was eventually consolidated to address the system requirements.

3.4.1 CFD simulations

The 3D CAD model was designed with FreeCAD v0.18.4. Grid generation, pre-processing and numerical solution of the mixing process in a stirred tank was executed with SnappyHexMesh grid generator and pimpledymfoam solver in OpenFOAM v3.0.1. Post-processing of the simulation dataset was carried out with ParaView v5.8.0. A Dell Precision 5530 Notebook (processor Intel(R) Core (TM) i7-8850H CPU 2.60GHz, 2592 MHz, 6 Cores, 12 Logical processors) with both Linux Ubuntu 16.04 and Microsoft Windows 10 as operating systems was utilized to run all relevant actions for the integration process. The simulation dataset was saved in the internal hard disk after the calculation was completed.

3.4.2 AR/VR technology

Developing an AR/VR application requires 3D computer graphics software to compile and build an executable final user application. Nowadays game

engines support AR/VR projects via software development kits (SDK) as cross-platform developers. Unity and Unreal game engines have wide compatibility with AR/VR SDKs (details in the Supplementary information for Chapter 3). It was decided that the best procedure for this integration study was to use a game engine with related AR/VR SDK. The AR application was developed with Vuforia SDK that was operated in the Unity 2019.1.0f2 game engine. A marker-based detection approach was selected to interact with the AR application with a real environment as being an easy-to-adapt feature. Vuforia SDK requires an online asset generation of marker for Unity. Although the present study was aiming to assess the integrity of the engineering simulation dataset, some of the interactive digital elements were also adapted to experience features of AR. Virtual buttons in Vuforia SDK were customized for use with the AR application to increase the users' interaction and immersion. Customization of the final-user console with either an AR or VR SDK does not affect the data processing procedure. A mobile application was generated with Unity and Vuforia SDK to visualize the simulation results into mobile marker-based AR. A Samsung A20e with Android Pie 9 was employed to test the final application.

3.4.3 Data processing

CFD post-processors are typically incompatible tools to process the CFD dataset throughout multiple platforms. Notably, these tools target visual representation of the dataset in a single or embedded platform upon engineering demands. Lack of 3D data export and connectivity options with external platforms is the main shortfall of CFD post-processors. The data format is one of the core elements of the system architecture along with the complete development procedure to store, extract, transfer, integrate and interact simulations with AR/VR. In order to identify the selection of an appropriate data format, a case study was performed. Blender v7.9. was implemented as a data processor to exchange data among 3D formats.

Assessment on simulation dataset

An exploratory research was performed (see the Supplementary information for Chapter 3 for details) to identify data import and export capabilities of software in use throughout multiplatform integration. Seven different cases were identified to assess the data import and export capabilities of software as shown in Table 3.1. In the scope of the present study, GLTF and WEBGL/VTKJS, newly developed mobile-friendly 3D formats for AR and web-based platforms [158, 159], were additionally taken into consideration.

Table 3.1: Case studies designed from data processing options supported through multiplatform integration.

Software Process	OpenFOAM Export	ParaView Import	ParaView Export	Blender Import	Blender Export	Unity Import
Case 1	FOAM	FOAM	X3D	X3D	FBX	FBX
Case 2	FOAM	FOAM	X3D	X3D	GLTF2	-
Case 3	FOAM	FOAM	X3D	X3D	OBJ	OBJ
Case 4	FOAM	FOAM	X3D	X3D	DAE	DAE
Case 5	FOAM	FOAM	GLTF1	-	-	-
Case 6	FOAM	FOAM	X3D	X3D	STL	-
Case 7	FOAM	FOAM	VTKJS	-	-	-

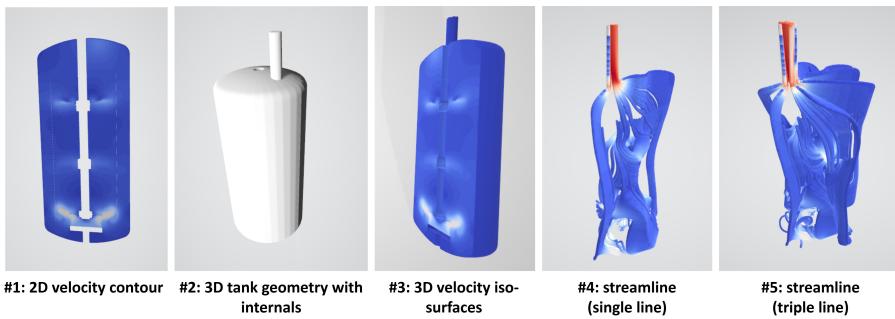


Figure 3.4: Visual representations of CFD dataset assessed in the case study.

Five different visual representations from the CFD dataset were sampled for the assessment (Fig. 3.4). Vector-based visualization was purposefully eliminated due to the same 3D data structure with volumetric visualization of streamlines. Initial cases were performed for each processing option to examine the intervention of visual representation techniques. Data size and processing times were compared for each case separately. Once the data processing procedure was finalized, the quality of data processing was qualitatively evaluated to detect whether any data was lost. Repetitions were prompted under conditions at which only the required software was run. Finally, additional tests and comparisons were performed to anticipate enhancements that could be entailed in the future with a focus on data processing.

Development of the end-user console

Integration of the CFD dataset with AR/VR was performed within the digital environment as illustrated in Fig. 3.5. End-user console was solely designed for the visualization of CFD dataset with mobile marker-based AR application.

Table 3.2 presents the dataflow diagram of the application built upon the system architecture as a transcript of the integration. The full transcript including system requirements can be found at the Supplementary information for Chapter 3.

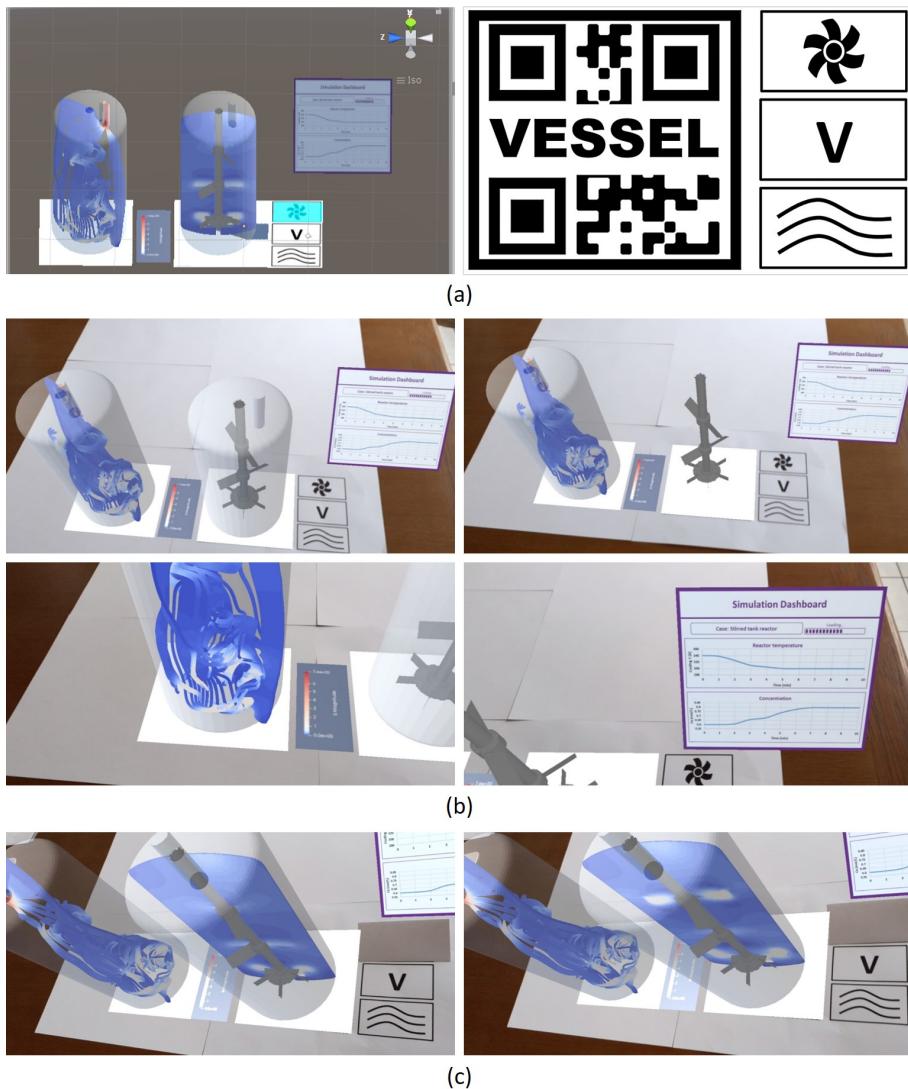


Figure 3.5: End-user console developed for mobile marker-based AR application; virtual design environment in the game engine and AR marker (a); scenes from the application (b); visualization of transient 2D velocity contour with virtual button (c).

Table 3.2: Dataflow diagram of the mobile AR application generated from the system architecture.

Component	Sub-component	Data analytics			Data coupling	
		Dataflow	Format	Size (MB)	Processing time (s)	One-way
Data creation	CAD	1	STL	2	-	-
	Pre-processing	2	FOAM	122	-	-
	Simulation	3	FOAM	4807	-	-
	Post-processing	4	FOAM	4807	-	-
Data processing	Database	5	FOAM	4807	-	-
	Extraction	6	X3D	85	4.8	Python in Anaconda
	Transformation	7	FBX	12	30.72	Navigator with required packages
	Virtuality continuum	8	FBX	12	-	-
AR/VR technology	Concept of immersion	9	-	-	-	-
	Perception	10	-	-	-	-
	Integration	11	FBX	12	6.5	-
	Interaction	12	-	-	-	-
End-user console	Built-in	13	FBX	12	65	-
	Simulator	14	APK	58	112	-

3.5 Results and discussion

3.5.1 Evaluation of extract-based data processing with suitable data formats: Case 1, Case 3 and Case 4

Complete integration of the CFD dataset with the game engine was only achieved with Case 1, Case 3, and Case 4. Even though the STL data exchange format (Case 6) could not be integrated into the game engine, it was also processed to assess the potential due to its widespread fame in computer-aided design (CAD). It should be noted that proprietary data formats do not reveal data encoding techniques. Hence it is hard to predict the behavior under varying circumstances. A comparison among relevant formats was therefore imperative to unveil data processing characteristics. Fig. 3.6 shows data processing analytics of the cases based on data size compression and data processing time. Each data presented in the analysis is the average of 10 repetitions with a 1.5% maximum error rate for the processing time. No change was observed in the data size. All other external and irrelevant activities were shut down and tracked with the total central processing unit (CPU) utilization in all cores, while the repetitions were carried out.

The comparison between the case studies highlighted that FBX, OBJ and STL reduced data size significantly whereas DAE unexpectedly increased it. Large volumes of dataset is a major trait of CFD simulation datasets. Allocating lower data size in computer memory is, therefore, a desired trend. As a higher-size data format would comprise more information related to the 3D assets, it could also be designed without concerns over an inefficient data encoding technique. The data processing time and the quality of data should be considered concurrently so as to make comparison reliable. A striking observation emerging from the data format comparison was the processing time. Interestingly, DAE processed the simulation dataset in a far shorter processing time: at least 1.5 times faster than STL, 3 times faster than FBX, and 7 times faster than OBJ. Though data size was increased with DAE, it required less processing time.

The study did not confirm any significant variation among the visual representation techniques of the CFD datasets shown in Fig. 3.4. All data exchange formats revealed a particular but similar data processing analytics for visual representation techniques. The larger the data size was, the longer the processing time became, as illustrated in Fig. 3.6.

The complete integration of the CFD dataset in the game engine included four major processing steps: export from ParaView, import to Blender, export from Blender, and import to Unity. Further analysis of the data processing time underlined that import and export characteristics of software differ among

data formats. In spite of a faster export from DAE with Blender, the import from DAE to Unity was slower than FBX and OBJ. As shown in Fig. 3.6b, processing times were compared among data formats through data processing. CFD visual representation techniques again did not reveal any noticeable difference. In all cases, OBJ required a longer data processing time compared to FBX and DAE. There was no significant deviation between FBX and DAE for CFD visual representations #1, #2 and #3. However, streamline-based CFD visual representations #4 and #5 took a longer time with FBX. This stresses the importance of an inclusive assessment concerning data format, data size, processing time, and software.

It is noteworthy that the data size and processing time are quantitative aspects of the integration. However, they are not related to the data quality. A further inspection should, therefore, be performed to assess data loss against relevant CFD post-processing (Fig. 3.4). To do that, the processed 3D data file was compared to the initial 3D data imported from the CFD post-processor. The study showed that both FBX and DAE import all relevant visual assets related to geometry, appearance, and the environment in a single file without any change. On the other hand, OBJ encoded the geometry and appearance in different files, and entirely excluded scene and animation. Despite the fact that the geometry was encoded without any data loss, encoding appearance in an external file caused a troublesome data import to game engine in which appearance was eventually lost. This can prevent practitioners to utilize the OBJ when appearance (color, legend, contour, etc.) is an essential part of processing. Caution must be exercised in the use of OBJ accordingly. Moreover, both FBX and DAE kept and encoded animation created with intermediate software while OBJ did not. Creating 3D animation with OBJ should be done in the final environment, for instance, the game engine itself. FBX and DAE further brought assets with layers at which enabling and disabling of particular visual contents could be performed. All three formats were open for scalability in the spatial domain.

Another comparison was performed for post-adjustment made in Unity and response time related to the data format used. Change of texture, scalability, and execution of manipulations were investigated. It was indicated that post-adjustments in Unity with FBX was 1.4 times and 5 times faster compared to DAE and OBJ, respectively.

The results point to the likelihood that each data format can enable unique characteristics to prompt data processing methodology upon data size, processing time, quality and post-treatment. Practitioners should decide on suitable data formats upon constraints of the multiplatform integration.

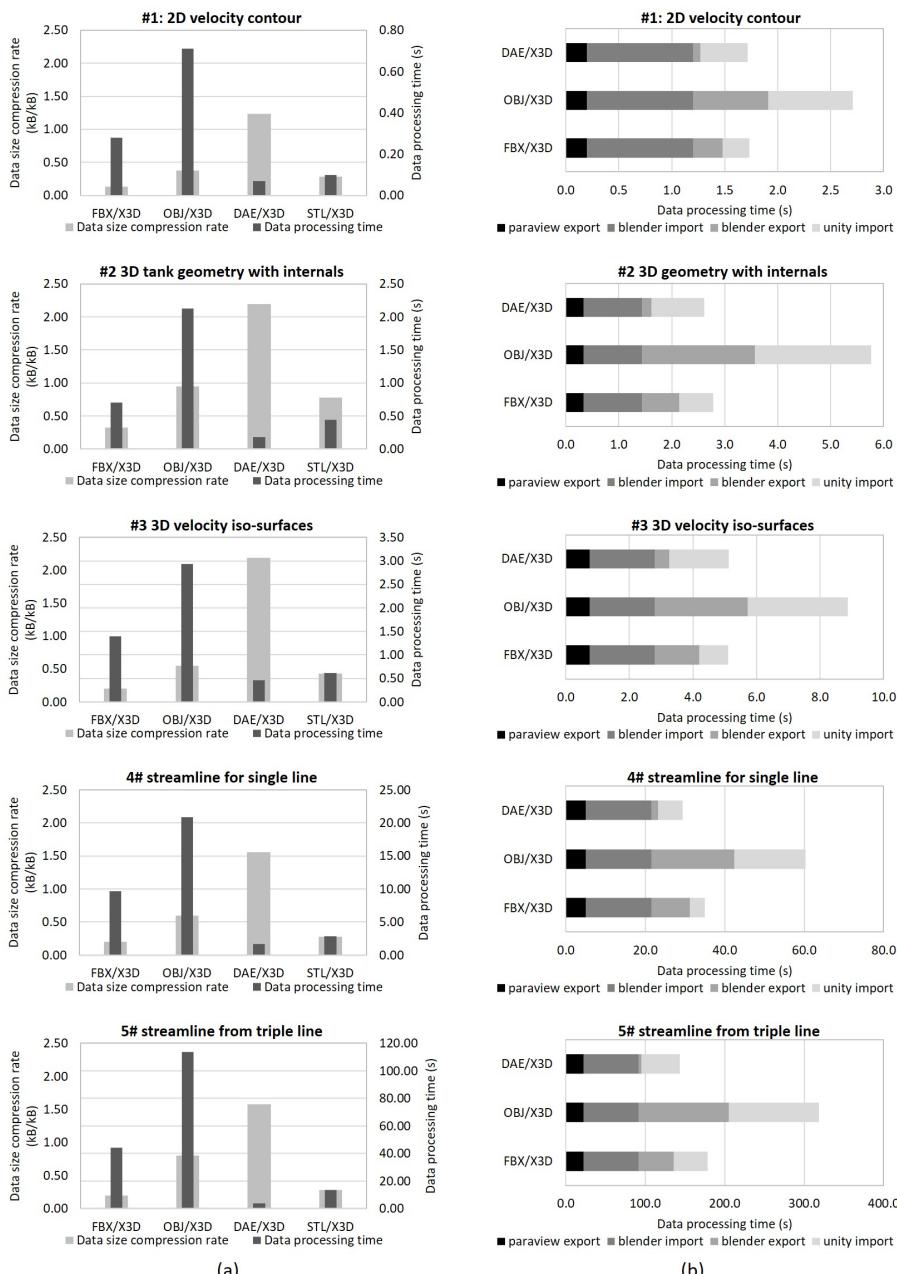


Figure 3.6: Data analytics of processing options; data size compression (a); data processing time (b).

3.5.2 Failed data processing options: Case 2, Case 5, Case 6 and Case 7

In this section, an investigation was elaborated on data formats for simulation datasets that would be potentially integrated into AR/VR in the future. STL has evolved to world-wide utilization due to the support of CAD software. Fig. 3.6 shows that data size and processing time were reduced significantly with the utility of STL against OBJ. The main downside of STL is no support of game engines, which makes its applicability impractical.

Comparison between software throughout the integration based on processing capabilities assured that X3D is the most convenient data exchange format to start with as it was applied in the present study. Moreover, GLTF1 and VTKJS data formats were also taken into account in separate data pipelines to assess data encoding performances. It was recently claimed that both formats could simplify data encoding procedure and shorten software pipeline [160, 161]. Another study stated that GLTF reduces complexity of 3D data and users' interaction, but also quality [159]. These formats currently cannot be a part of data processing options due to the lack of technical support from game engines. Nonetheless, concerning an update of the support in the future, we performed a comparison between the 3D data exchange formats X3D, GLTF1 and VTKJS as illustrated in Fig. 3.7. Both data size and processing time were clearly reduced with GLTF1 and VTKJS. Even though both data formats concluded promising results, the currently released versions of game engines do not give any official support. Hence, the quality of the data processing remains unanswered.

The CFD dataset was processed to the GLTF2 data format with the use of Blender as proposed with Case 3. It surprisingly resulted in far adverse analytics: 5 times higher data size than FBX and 47 times higher data processing time than DAE. The data format was also not officially supported by game engines.

ParaView v5.8. extended its data saving option, including the OBJ format, as an ASCII data type. This enables an alternative data processing methodology, directly from ParaView to Unity without the use of any intermediate 3D computer graphics software. Despite this direct connection, several drawbacks come along with the integration. Firstly, ParaView uses the OBJ format to store data rather than as an exchange format. This, therefore, prevents multiple data processing at the same time. Moreover, it was observed that 3D internal mesh cannot be saved with OBJ. Visual representations #1 and #4 were solely possible to process with OBJ. Also, due to the data format characteristics, OBJ only includes geometry in the main file. Compared to Case 3 in which OBJ transformed from X3D, the dataset can be transformed with at least 1.4 times higher data size compression and 3.1 times faster processing time.

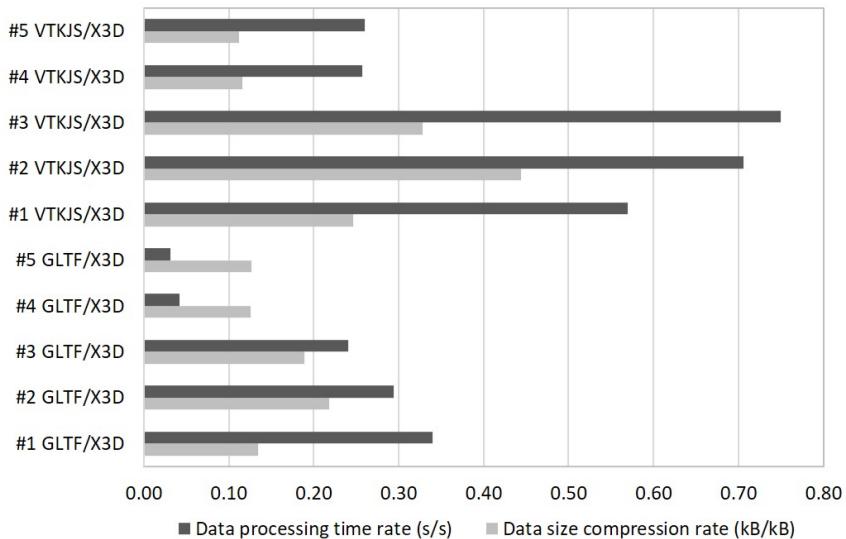


Figure 3.7: Data export comparison among X3D, GLTF1, and VTKJS.

Researchers should always keep an eye on recent developments in 3D data formats and software. Unofficial data import and export source-codes could be a remedy to carry out a process with targeted 3D data formats. Nonetheless, a thorough examination should be done on data analytics and quality in order to make integration reliable.

3.5.3 Data and workflow: automated data processing

One of the key advantages of the system architecture is the detailed data and workflow of the development procedure as shown in Table 3.2. Whereas the system requirements provide features to prescribe given tasks, they also allow for suggestions on which enrichments could possibly be applied to the system components. For instance, the targeted hardware for the end-user console could be incompatible due to the requirements applied in another system component or vice versa. In this regard, the component-oriented trait of system architecture can provide a sustainable development strategy by reiterating development procedures upon the workflow. The data processing approach does not only serve for OpenFOAM, but also COMSOL Multiphysics, Ansys and Siemens Star-CCM+ can be tailored in the processing via compatible data formats (details in the Supplementary information for Chapter 3 for details).

Communication among digital platforms can provide bridges to execute sub-components in an automated scheme. The data processing encompasses multiple manually driven steps that must be set by the practitioners as demonstrated in Table 3.2. In the framework of the present study, bridging between the CFD post-processor and the game engine was achieved to automate data processing based on methodologies M1 and M2 (Fig. 3.3). Fig. 3.8 illustrates an algorithmic approach on how to generate a baseline and configure the scheme for an automated process. Either a python state (M1) or data extracts (M2) can be entailed into the automated data processing approach. Once a baseline is generated, any data produced by a CFD solver can directly be processed and integrated to game engine via a data processing script develop in the present study. The automated processing would seem to imply that whole post-processing and data processing workflows can be standardized and provide a rigorous connection. Practitioners can accordingly customize the procedure upon the system requirements with minor changes in the data processing script.

A blueprint of the data processing script developed in the present work is detailed in Fig. 3.9. It essentially provides a simplified, optimized and automated one-way coupling procedure between CFD data and game engine. An input file of CFD data, either a python state or extract, should be set by the user before running the script. The full script was developed in Python with Spyder in Anaconda Navigator utilizing the packages ParaView v5.8. and Blender v7.9. It has capabilities to process both steady-state and transient CFD datasets to generate visual CFD simulation data, supporting multimedia files (e.g. colormap in image format), analytic data, and data processing performance. The custom Python code developed in this work is available in the project's GitHub repository: https://github.com/sersolmaz/CFD_AR_VR.

It is noteworthy to mention that the platforms entailed in the data processing script should be consistent in terms of released versions to run a coupled dataflow without any disruption. Practitioners can take advantage of automated data processing due to the reduced complexity in data processing and the dataflow. They may further benefit from outsourced tools such as external databases provided by research institutions and simulation companies to process and adapt digital content freely available.

In the next phase, a two-way coupling between the data creation and the end-user console would provide a fully automated integration. This could allow users to manipulate existing conditions and produce new simulation results actively from an optimized CFD workflow. The proposed data processing script originally complies with two-way coupling approach since nothing changes in the data processing approach from CFD solver to game engine. The users' interaction in the digital environment with simulations could be achieved in various techniques based on sub-components and system requirements. As an

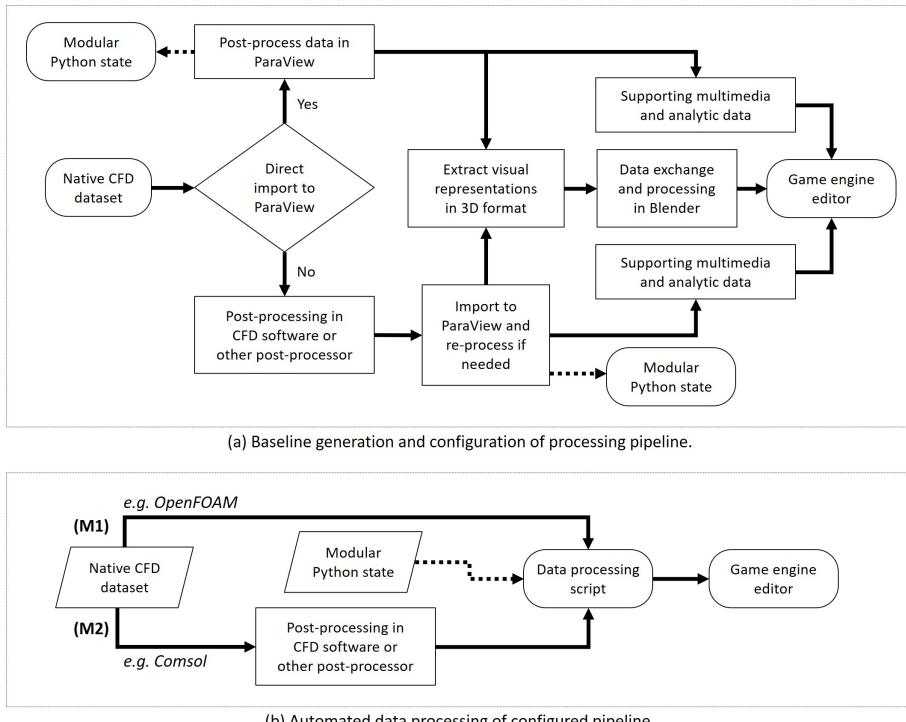


Figure 3.8: An algorithmic approach on data processing; baseline generation (a); automation of methodologies M1 and M2 (b).

example, manipulating one of the boundary conditions in simulations could be done via hand-held devices, touch screens, image processing, IoT devices, system-on-chip, voice commands or any other methods that have so far been developed, as well as considering high-tech connection opportunities such as ubiquitous computing.

3.5.4 Data management

Both commercial (Ansys, Comsol, and Star-CCM+) and open-source (OpenFOAM) CFD solvers were found to be designed based on well-structured data management systems. Similarly, game engines also relied on management systems to compress and retrieve the data in use. A processed CFD data imported into Unity is automatically stored under a related assets directory

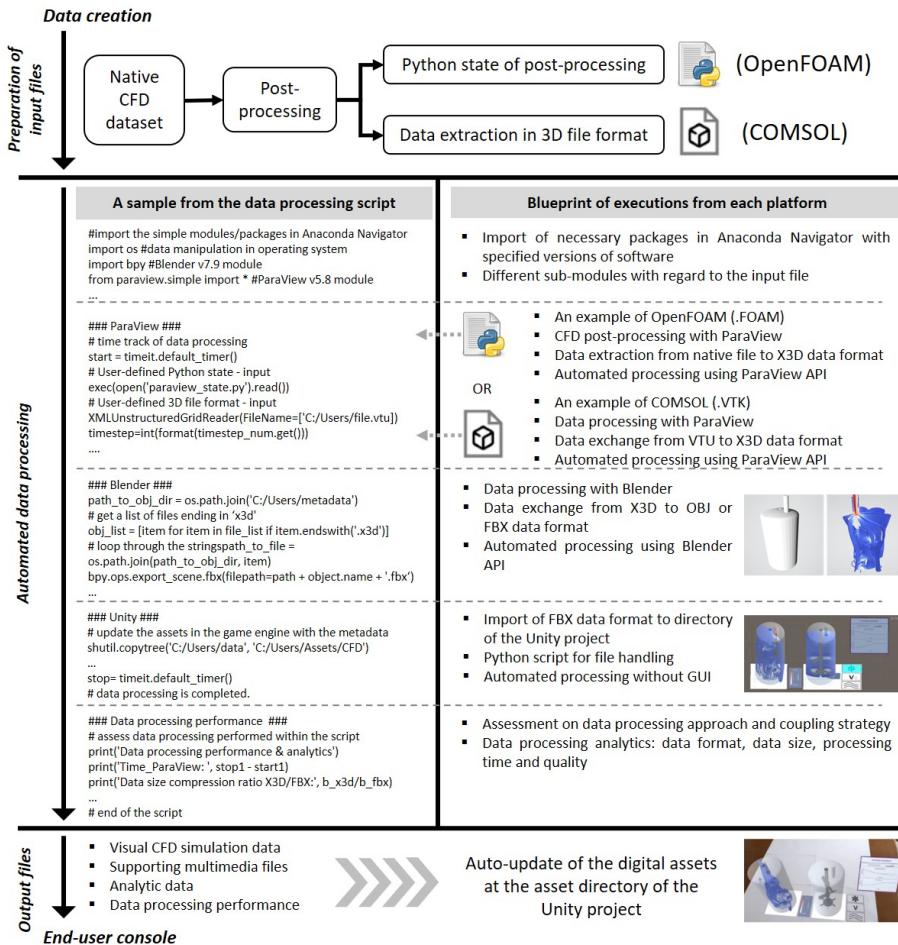


Figure 3.9: Automated data processing script from data creation to end-user console and the blueprint of the entire procedure.

Table 3.3: Comparison among data models to store and retrieve CFD dataset with ParaView.

Data model	Reduction in file size (%)	Data saving time (s)
VTM	53	0.2
VTM (zip)	77	13.4
CGNS	29	0.8
CGNS (zip)	75	27.2
XDMF	63	9.3
XDMF (zip)	77	16.5
OpenFOAM native file (zip)	27	4.3

where the project was initially created. Surplus and repetitive metadata generated throughout the processing should be avoided to keep the data size of the final application optimal. Processed data is only stored in the game engine and the final application. Therefore, all desired CFD post-processing should be determined in advance.

In case a new CFD post-processing is to be integrated into the final application, the system should be able to access the native CFD data which is generally large and complex. Instead, extractions from native CFD data into manageable parts can alternatively serve while reducing data by orders of magnitude as previously mentioned. Extracted CFD datasets should be encoded by using a convenient data model to store, retrieve, reproduce, and reprocess metadata in a secure routine.

A study was initiated to examine data size, data saving time, and retrievability of data storage formats supported by ParaView. A particular time step with a size of 339 MB from the CFD results of the stirred tank reactor was sampled for the comparison. Table 3.3 shows the reduction in file size against the native CFD dataset. Whilst the smallest data size was reached with XDMF, the shortest operation time was achieved with VTM. All data formats enable us to retrieve CFD data in ParaView without data loss. Further reduction in data size was also achieved with traditional data compression type ZIP. CGNS, VTK, and XDMF gave satisfactory performances on data size and saving time. A database system might be developed to manage CFD parts intelligently using one of these formats whereas a frequent use of the data is targeted.

3.6 Strengths and weaknesses

Literature overlooked technical challenges related to the processing of simulation data among cross-platform development tools, as being an inter-disciplinary concern. Researches carried out to date suffered from stand-alone, platform-specific, computationally-demanding, non-replicable, and manually integrated data processing methodologies. This hindered developers to consider AR/VR tools to visualize CFD simulation data. Our study provided a detailed technical examination regarding the integration of CFD simulation data with AR/VR applications. We developed an extract-based data processing methodology with lightweight, easy-to-implement, end-to-end, automated and free-to-use utilities. The academic community can readily benefit from our study to evaluate the best scenarios to implement CFD simulation data with AR/VR tools. Not only CFD simulations but also any type of visual data processed with ParaView (or any other post-processing software supporting suitable data formats) can be integrated into the workflow presented in this study.

The present study only investigated commonly used software and data formats in the multiplatform integration based on the feasibility study conducted prior to our investigation (see the Supplementary information for Chapter 3 for details). Due to the scope of our work, we did not provide any information relevant to the validation of CFD simulation results, which is essential to present accurate information. Likewise, except for virtual buttons in AR application, we obscured human-computer interactions, which are normally considered to be one of the fundamental features of AR/VR by means of immersion.

In terms of the challenges for future research, this study concentrated on the integration of CFD simulation data with AR/VR development tools; however, more research is required in this area in order to remotely update integrated data in final user applications. Also, it would be interesting to investigate newly adapted lightweight data formats to reduce data size and increase data processing speed while preserving quality.

3.7 Conclusion

The present work proposed generic system architecture and examined methodologies on the integration of CFD simulations with AR/VR. The results indicated that the system architecture has a promising utility to prescribe a development strategy. The study provided a generic design pattern as well as miscellaneous workflows to develop educational tools with CFD and AR/VR. Extract-based processing of CFD dataset highlighted a simplified integration

that the practitioners can readily pursue. A comprehensive investigation was also performed to evaluate data processing methodologies on their data format, size, processing time and quality. Findings showed remarkable possibilities to overcome ambiguities related to data process options in the literature. The present work also disclosed an automated dataflow between native CFD dataset and the game engine. A descriptive guidance on the management of data in use additionally demonstrated to manage large CFD data parts.

In this study, we focused on a rigorous integration that can help practitioners to maintain long-lasting digital tools with rapid and easy-to-update features. Future work will concentrate on two-way data coupling and technical works to prototype such digital tools. User assessment studies will be performed to assess both digital tools and implementation in engineering education.

Chapter 4

Interactive CFD simulations with virtual reality to support learning in mixing

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Author contributions: S. Solmaz conceived the research, performed the data analysis, interpreted the results and wrote the article. T. Van Gerven contributed with his guidance and expertise in this work.

Abstract This study presents a user-friendly digital learning environment with interactive computational fluid dynamics simulations for higher education in chemical engineering. A client-server network is introduced to maintain an automated two-way connection between multiple CFD solvers and a game engine as a cross-platform development tool. A modular software development approach is pursued to obtain long-lasting connected digital applications. To prevail over heavy calculations and standalone features, a content delivery network is structured, through which any end-user devices are made employable regardless of hardware performance. From desktop to virtual reality applications, multiple digital platforms are demonstrated within a case study of mixing. The system performance of technical integrity is assessed to ensure a feasible and effective connection through the client-server network. A task-centered educational model

is implemented to design digital learning environments concerning complex skills to be developed by learners. Discussions are drawn upon the applicability of the system with respect to traditional teaching practices.

4.1 Introduction

Digital devices are becoming an intimate part of learning since the turn of the century. European Union has declared several research plans to adopt digital resources in education and training [162], including a recently debuted Digital Education Action Plan for 2021-2027 [8]. The plans have been proposing concrete steps to lead to a high-performing digital education ecosystem with digitally competent human resources. Principally, high-quality learning content and user-friendly tools have been strictly underlined together with the emergency of augmented and virtual reality (AR/VR) technologies.

Chemical engineering content is ever-evolving to find efficient processes. Notably, process intensification has been receiving much attention in recent years from academicians and industrialists [163, 164]. Mixing is one of the core unit operations in chemical engineering taking part in almost every chemical process. For instance, in order to develop a millifluidic crystallizer to produce pharmaceuticals within an efficient process, an engineering student should be able to comprehend and interpret transport phenomena, multiscale and multiphysics interactions. Not only handbook solutions and experimental studies, but also multiphysics computational fluid dynamics (CFD) simulations can be blended in the technical work to make progress in an efficient manner [121].

CFD simulations are essential tools to support engineering design and analysis. Cost time benefits, advanced data exploration and fast prototyping are the main advantages of CFD simulations. A deep understanding of physical, mathematical and computer science is critical to obtain optimal simulation workflows. These require physical accuracy, optimal calculation time and meaningful result extraction. CFD simulations have a dynamic role to play in engineering education, by producing abstract learner content, and facilitating active learning environments [12]. However, neither lecturers nor students might be acquiring relevant skills to deal with the complex nature of simulation environments. CFD is generally assumed not to be user-friendly and does not provide supportive content in the context of instructional design. Engineering students can face a high entry barrier in simulation environments developed through conventional workflows.

Game engines have recently shown great potential to develop functional and high-purpose digital environments from mobile to AR/VR applications. In essence, they can effectively serve in the development of head-mounted display (HMD) VR environments where the learning experience is assisted and assessed with simulations and supportive information. These applications can also amplify cognitive skills with advanced human-computer interactions (HCI), while leveraging motivation within user-friendly, fun and engaging environments. A recent study reported that process simulations in a VR environment increase students' proficiency in chemical engineering content [165]. Integration of CFD simulation data with game engines has already been demonstrating applications including positively responded user assessments [105, 166, 117, 118, 36, 119]. Despite this, user applications are still lacking functional, well-performed and easy-to-implement design elements in the development workflow. Several key challenges are present to adopt AR/VR with technical content in engineering and education [109, 16, 17]. Digital applications are generally hardcoded, platform-specific and standalone, comprising a static CFD post-processing without any connection to a CFD solver or data processor [16]. Technical integration of simulation data with cross-platform software should still be studied to obtain long-lasting digital applications concerning software development workflow, remote connection, data visualization, and user assessment [17].

Taking on these challenges, this work develops an automated two-way connection between CFD solvers and the Unity game engine. In this study, the term two-way coupling refers strictly to a dynamic connection between CFD solvers and user applications built in Unity. The ultimate goal is to develop CFD simulation-assisted user-friendly digital applications to teach mixing in chemical engineering. Whilst the system ensures content-wise accurate and rich environments, it can support life-long learning, enabling simulation-driven learning cycles as supplementary tools to traditional applications. The present study demonstrates significant contributions:

An automated two-way connection between CFD solvers and Unity to perform interactive simulations. A remote content delivery approach is presented with a client-server network model. The integration is strictly tied to modular, automated, easy-to-update, lightweight, end-to-end and open-source utilities. Both OpenFOAM and COMSOL are simultaneously and successfully connected to Unity. Seamless integration is prompted between CFD software and user applications. Automated workflows are extremely flexible and easily be customized for any compelling needs with the modular architecture.

Well-maintained features to interact with CFD simulations in VR. User interaction and system performance are ensured to obtain a feasible development workflow concerning data processing, dataflow, data management and delivery systems in the network. The system also highlights practices

to develop co-simulation and digital twin environments with interactive CFD simulations remotely accessible.

A digital authoring tool to customize the learning environment with CFD simulation data. Thanks to the game engine, the digital environment can be quickly customized upon developers' needs on digital learning content, as well as user interaction and device. A task-centered educational model is implemented to design a digital learning environment based on complex skills to be developed by learners. A VR application is configured to learn macroscale mixing through the analysis of a stirred tank reactor with CFD simulations.

4.1.1 Background and review

Early research in this field primarily focused on the automation of CFD solvers to produce data for cross-platforms, rather than two-way coupling. Challenges related to a fully coupled computing system stressed the need for an expert to maintain automated data generation and simulation routines [30]. Recently published works mostly studied remote connections to automate CFD solvers to produce data for cross-platforms. Studies reported the importance of pre-optimized models in CFD workflows with constrained parameters that non-expert users can easily interact with [167, 113]. Several remote connection models were also exhibited to maintain semi-automated routines for CFD solvers and data processing [31, 32, 33, 34], including peer interaction [34]. These studies tended to focus on the domain- and platform-specific applications with hardcoded elements in their systems, thereby posing a danger to be outdated in a short period of time. Above all, manual expert interferences were still required in most cases of two-way connections.

A review of the literature on this matter reported that technical works generally lack automation of dataflow between CFD solvers and user applications. The study further stated that digital environments were built upon very particular data processing methodologies that make any post-production unfeasible due to hardcoded utilities [16]. Recently, a one-way automated connection was proposed to integrate CFD simulation data with game engines [168]. Even though a methodology was presented toward a two-way connection, the study mostly investigated robust data processing work rather than connectivity.

Technical works related to fully automated two-way couplings between CFD solvers and cross-platforms have been gaining momentum to develop digital tools for non-expert users. Shi et al. proposed a well-maintained network to perform interactive CFD simulations with virtual reality. User interaction with simulation data and dynamic post-processing were suggested through very plausible approaches to bring case-specific but easy-to-customize features [36].

One of the major drawbacks to adopting this system is the CFD solver in the maintained connection. A Lattice-Boltzmann solver was implemented to run domain-specific CFD simulations for cardiovascular science, which is based on a specific software architecture different than the ones used in CFD solvers such as OpenFOAM, COMSOL, Ansys and STAR-CCM+. Another study took on the difficult task of the automation of the whole process in a digital twin model. It proposed an automated connection utilizing a CFD software architecture that is similar to commonly used ones in academia and industry [169]. Particularly interesting was the way in which the study additionally detailed the automation in-depth with a dataflow presented. A user application was presented targeting non-experts to perform CFD simulations with constrained input parameters. However, the automated routine was built toward a digital twin approach, and the system did not consider either immersive technologies or game engines. There is still considerable ambiguity to maintain an automated two-way connection between commonly used CFD solvers and Unity.

User interaction with simulation parameters was discussed by a few scholars. In general, parameter-based interaction was preferred to acquire user input [170, 169, 36]. In some cases, manipulation of model geometry with different HCI interfaces was even taken into account implementing hand controllers, haptic devices and image processing. Studies recommended considering HCI interfaces with caution concerning accuracy and steadiness of geometric manipulations made. Limiting user interaction and adding supportive features were found to be an optimal approach to automate systems such as local grid refinement and pre-modeled geometric extrusion. Expert support was strictly mentioned in the development of automated systems to overcoming technical issues that might affect CFD simulation workflows [169, 36].

Dynamic post-processing of simulation data in the user application was investigated to facilitate a constrained but flexible data exploration tool for non-expert users such as slicing, clipping and animating [170, 32, 36, 171]. While the authors' position is that the connection is feasible, there are many weaknesses in this concept of which a recent criticism was the following [17]. Either a game engine or user application is employed to process CFD data which is often computationally demanding for end-user devices. Relevant post-processing algorithms to process CFD datasets should be re-coded in the game engine, mainly from the ground up.

Furthermore, cross-platform environments with real-time CFD models have become common in academia [123, 118]. However, the current state of the research only promotes either very simple or low-fidelity simulations. These would only seem to be helpful in teaching the basics of fluid mechanics.

Lastly, the use of a functional mock-up interface (FMI) is a standard approach

becoming popular in the context of interoperability. It is fundamentally a communication hub to manage connections with a common application programming interface (API). The FMI standard is an open-source format enabling co-simulation and model exchange features among heterogeneous platforms. A software should give support on the FMI standard to be tied in a connection pipeline. No study has been found in the literature developing a two-way connection with FMI within the scope of the present work. COMSOL [172] and OpenFOAM [173] do not directly give support on the FMI standard yet. In our proposed approach any software with any type of API can be integrated with API-based modular connections.

4.2 Methodology

4.2.1 System design: the client-server network

The present study proposes a client-server network to maintain an automated two-way coupling between CFD solvers and user applications. This approach aims to develop user-friendly learning environments with technological advancements. A client-server network is a distributed system in which servers and clients are given specific tasks to maintain a remote connection. Once the client initiates a request, the server receives the request, executes the necessary action, and then responds back to the client. Multiple clients and servers can be implemented to the same network in case the system requires heterogeneous utilities, for example, high-performance computing (HPC) facilities for computationally demanding tasks. The client-server network typically adheres to an internet protocol suite (TCP/IP) with connected utilities.

Fig. 4.1 presents a client-server network to establish a two-way connection between simulation software and game engine. To achieve this, we propose two subsequent workflows; *design* and *automation*. The network provides a flexible environment in which multiple users connect and interact simultaneously. All heavy-duty processing works are executed on the server-side. The client hardware, which employs the user application, is merely utilized to stream the content delivered through the network. The entire network is maintained by the following five executive modules: user application, computational fluid dynamics simulator, simulation datasets, data processing software and game engine. Datasets and data processing software modules are adopted from our previous work to integrate CFD data with Unity [168].

The network consists of one built-in and eight inter-connections as numbered in Fig. 4.1, whereby in-house Python scripts automatically handle actions

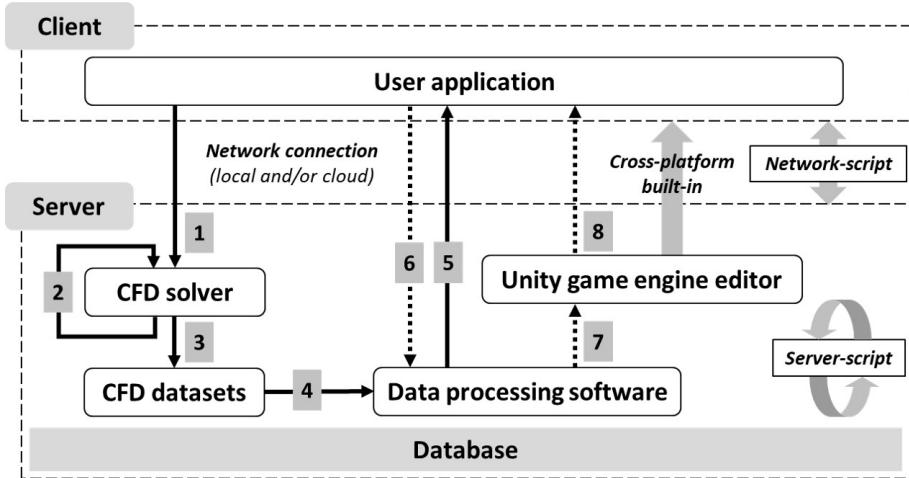


Figure 4.1: The client-server network to maintain an automated two-way coupling between CFD solvers and user applications developed with Unity. Connections with dashed lines are optional dataflow pipelines that might be entailed for advanced interactions.

inside the network. The server-side is managed via *server-script* to maintain communication among the modules. In comparison, the client-side does not require any script as all essential settings are fixed within the cross-platform built-in. Interaction between the client and server is handled with *network-script*. These in-house scripts are mainly composed of file handling operations with standard Python libraries.

The *design* workflow is the phase in which a user application is built in Unity only one time. Decisions are made in this phase to draft a baseline connection (from 1 to 5) with intended optional features (from 6 to 8). Updates in user applications proceed with a content delivery network (CDN) created in Unity and then embedded in the client-server architecture. This avoids the requirement for the system to rebuild a new user application each time if the digital content is updated. Any content in the user environment can be remotely deployed as long as being linked to the CDN.

The *automation* workflow comprises fully integrated modules. It mainly includes all inter-connections without a built-in. First, the user input in the client is processed in a case file, which is sent to the relevant CFD simulation tool. This case file is then automatically updated in the relevant directory to run a new simulation. Results are saved in native formats and processed further to

integrate CFD data into Unity within third and fourth connections. Finally, the data in the user application is updated through the fifth connection. This way, a baseline automated two-way connection is achieved between CFD solvers and user applications.

Furthermore, the client can dynamically post-process simulation results through a restricted well-maintained connection between the user application and data processing software, labeled as the sixth connection. Likewise, a CFD solver is generally composed of a set of manual steps that must be accurately handled by an expert. Complete automation might be challenging due to the software architecture and data encryption in CFD solvers. Hence, an internal connection is separately demonstrated to CFD solvers, to stress the significance of automation using the second connection. In addition, in case the game engine is applied as an intermediate data processor, the seventh and eighth connections can optionally be established without built-in. For instance, to efficiently manage extract-based CFD data in user applications, a pre-processing via addressable asset manager in Unity might be tailored in the workflow.

The network is aimed at heterogeneous and distributed computing facilities, such as could and HPC servers. A database management system is prescribed to intelligently orchestrate data-in-use. All computationally intensive and complex data processing tasks are executed in the server. The data in the user application is kept in either the client hardware or database in the server. Each module in the server is inherently connected to the database at the back end.

4.2.2 Design of the learning environment

Performing CFD simulations requires complex skills to solve engineering problems. Learning in conventional simulation environments often happens by learning-by-doing. The environment does not comprise any assistance except help options relevant to the usability of the tool. This methodology has been heavily criticized by educational scientists and found less efficient than that of traditional instructional designs [76]. Meanwhile, game engines are versatile tools to develop a digital environment in varying contexts. Any assistance can be effortlessly delivered in runtime through guided learning environments.

Several interesting models to design digital learning environments have been researched by educational scientists over the last two decades. The four-component instructional design (4C/ID) model has gained much attention to support complex learning environments in numerous disciplines [69]. The model promotes four major components to enable complex learning; learning task, supportive information, just-in-time information and part-task practice. The learning environment in this study (Table 4.1) is originated from the 4C/ID

Table 4.1: Implementation of 4C/ID with CFD simulations; an example from a specific learning task.

Component	Principle	Generic content	Example
Learning task	Sequential	Intensification of mixing process in a stirred tank reactor	Assess different rotating impellers in a mixing process
Supportive information	Multimedia	Explains how to interpret simulation data of a specific task	Visual and written information about power draw and shear force
Just-in-time information	Signaling	Step-by-step, timely instructions to present procedure	Highlighting a component in the model
Part-task practice	Recognize-edit-produce	Improve performance on routine aspects with additional practices	Check mesh quality after geometric manipulations

model utilizing suitable design principles elaborated in the relevant research [69].

In particular, the learning task is organized toward the sequential principle to progressively increase complexity. A tuning approach is pursued to reduce the level of assistance given with supportive and just-in-time information throughout tasks. A smooth entrance, with a tutorial-like simplified very first level, is provided to let students explore the learning environment and usability in the first place. The complexity is then leveled up by tuning working memory and cognitive loads upon components of the model. The part-task practice is considered to improve performance on routine aspects of learning tasks in the simulation workflow. Besides, we also try adapting the following approaches to use multimedia effectively in the learning environment. The multimedia principle is mainly applied prior to the VR experience to give supportive information through pictures and animations with explanatory texts. The signaling principle is implemented for just-in-time information, in which instructions are highlighted in a step-by-step fashion upon the relevant step in the learning task. No study has been found in the literature implementing a task-centered complex learning method with CFD simulations in a digital environment.

All in all, it is likely that the 4C/ID model can help students to comprehend and operate simulation-driven learning environments easier than learning-by-doing. Students may develop necessary proficiencies as expected from engineers who deal with CFD simulations; remember, understand, apply, analyze, evaluate and create in a limited period of time [61, 12].

4.3 Implementation

This section details the development of connections in the client-server network. Two-way coupling between CFD solvers and Unity was demonstrated. Both OpenFOAM and COMSOL were tailored in the automated workflow. A case study was prototyped to assess the implementation including desktop, mobile, and virtual reality applications. The software packages developed in this study are freely accessible in the Supplementary information for Chapter 4.

4.3.1 Input from user application to CFD solver

Depending on the end-user device, the user can interact with the application through miscellaneous options. Touch screens, hand controllers, haptic devices and many others may be equipped to acquire inputs from the user. These interactions are directly adjusted in Unity regardless of the CFD solver.

Built-in parametric connections

User interaction with simulation data can be maintained using a case file that is exported from the CFD solver. A case file, also known as a system file, is a collection of sequential steps executed in the CFD solver written in a suitable API format. Any parameter in the case file can be externally adjusted. By importing the case file in the CFD solver, a simulation can be automatically run without any manual interferences. This approach enables a modular workflow to develop automated routines. Thus, the connection in the network was maintained based on case files exported from CFD solvers. First, a case file from a particular simulation was exported from the CFD solver. It was then embedded in Unity and linked to the user application's graphical user interface (GUI) for intended parameters. A file operation was ordered to process the user input in the relevant line and update the case file in runtime. In Unity, the operation was internally handled with a C# script, named as *ToTextFile.cs*. Finally, the updated case file was transferred to the server via *network-script* to perform a new simulation. Fig. 4.2 shows an example of the file operation in

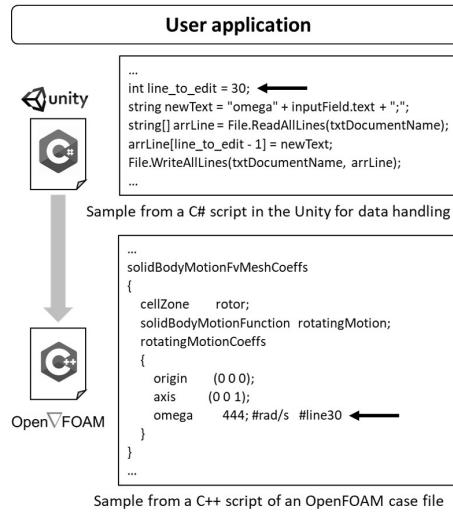


Figure 4.2: Processing the input into OpenFOAM simulation case file which is embedded in the user application built in Unity.

Unity to process input data into an OpenFOAM case file. A parameter-based approach was intrinsically taken into consideration to process the input from the user application.

Fig. 4.3 illustrates an overview of the implementation of both OpenFOAM and COMSOL case files in Unity. A modular connection was achieved without any hardcoded element in the dataflow. The *network-script* and the CDN settings in the game engine automate data transfer inside the network. It is noteworthy to mention that geometry models utilized in CFD simulations should be thoroughly logical, precise and stable to create and update a proper grid structure. Hand controllers and haptic devices can be still troublesome to accurately manipulate geometric features in the spatial domain [170, 36]. Therefore, the acquisition of input data through embedded user interfaces was mostly maintained with the parameter-based approach. This methodology sufficiently serves in the development of simplified, content-specific and flexible GUI for any CFD simulations, whereas non-expert users can readily adjust input parameters.

Geometry and mesh specific external connections

Skilled users may prefer an interactive freestyle fashion to manipulate geometric features. Although Unity does not provide any 3D modeling toolbox by default, the software has a modular structure supported by external toolboxes for 3D modeling. As can be seen in Fig. 4.3, we proposed two external connections for advance geometric operations in the system. The prior is for plug-ins such as ProBuilder and PIXYZ that can be imported into Unity for advanced runtime geometric operations. The manipulated geometry file should be exported in a 3D file format suitable to CFD workflows of COMSOL and OpenFOAM. The geometry is accompanied by a case file to integrate manipulations into the automated CFD routine.

COMSOL has a built-in geometry module to tackle geometric operations inside the software which can internally process both built-in parametric and external connections. In contrast, features in OpenFOAM, such as `blockMeshblock` and `snappyHexMesh`, enable a limited interaction to edit and update geometry directly in the case file, as handled with the parameter-based interaction. The geometry is generally hardcoded with predefined nodes and edges. This method can be problematic to process 3D and complex geometric modifications. Hence, the latter option, called the parametric geometry, is specifically dedicated to OpenFOAM within an open-source workflow to handle advanced geometric manipulations. An intermediate computer-aided engineering (CAE) software should be tied up to process geometric changes automatically. A complete connection was maintained by employing SALOME which is an open-source 3D modeling and meshing software. The software has an extensive Python API enabling various parametric operations to remotely reprocess geometry and meshing from a Python script. Initially, a geometry model with a grid structure was created from the ground up, and the project was saved as a dump study which collectively and sequentially writes all operations taken by developers into a Python script. As applied for built-in parametric connections, the Python script was embedded into the user application to process runtime interactions. This enables developers to prompt fully coupled geometry and meshing modules for OpenFOAM simulations. Any user-defined parameter processed in the Python script of a dump study can be automatically reproduced from the batch in the automated workflow. It is noteworthy that Salome exports meshes in UNV format that should be converted in OpenFOAM with `ideasUnvToFoam` utility. Besides, automation in the system can be straightforwardly expanded utilizing Python API of SALOME, for example, creating an automated grid convergence study.

Furthermore, Blender, a 3D computer graphics software, can be considered to maintain a modular, API-based connection for geometric operations. This

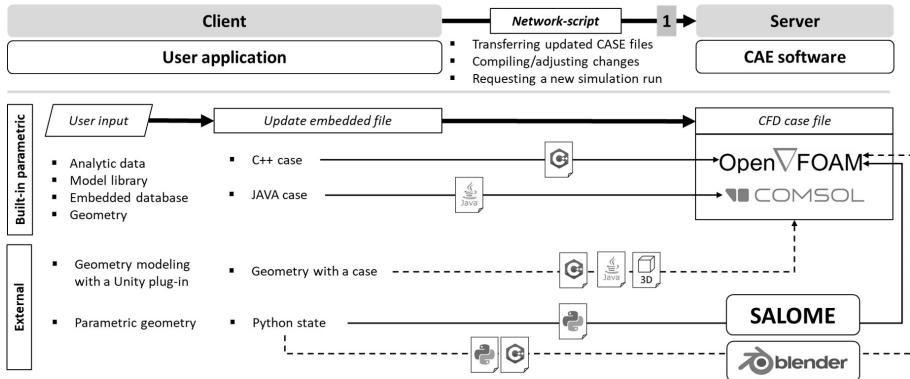


Figure 4.3: Built-in parametric and external operations to acquire the input from the user applications throughout modular and API-based connection. While continuous lines promote direct connections maintained in the study, dashed lines illustrate potential alternatives.

connection can convert geometry data to formats readable by Unity. Utilizing the Python API of Blender, an interoperable connection can be developed in which the input is processed in a Python state file embedded in the application. The connection requires external meshing software to recreate grid structures. In this study, instead of maintaining a working implementation, the connection with Blender is only to highlight the flexible structure of the two-way coupling strategy which enables developers to integrate and readily switch among various platforms.

4.3.2 Automated CFD routines and data extraction

Similar to calculations in the CFD simulation workflows, pre- and post-processing are also considerably time-consuming and iterative steps. Once an optimal workflow is decided by an analyst, pre- and post-processing steps turn into repetitive tasks that can be automatically executed. An automated CFD workflow with restricted options should be carefully prepared to control stability, precision and quality. The second connection in Fig. 4.1 points out to automated routines of OpenFOAM and COMSOL connected to the user application. Software-specific settings are essential to obtain inherently automated routines of each solver such as local and adaptive grid refinement, grid quality control, and many others commonly utilized in semi-automated CFD workflows.

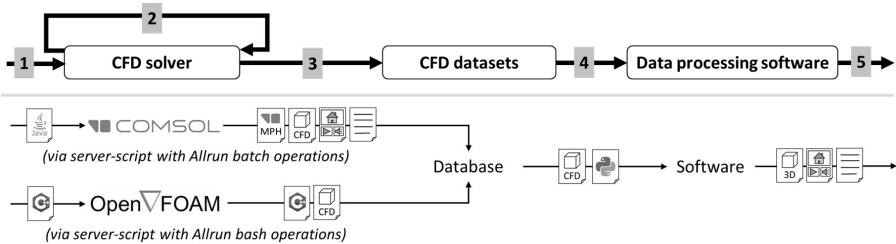


Figure 4.4: Automation of CFD routines and processing of data throughout the modules in the server.

Pre-processing, calculations, post-processing, and data extraction are the main steps sequentially executed in a typical CFD simulation. A fully automated CFD routine can be maintained with a script to execute each step from the relevant directory. Fig. 4.4 depicts automated routines for each solver with detailed workflow diagrams. The *server-script* manages the utilization of command scripts to automate the workflow, batch processing in Windows and bash processing in Linux operating systems (OS).

Automation of data extractions should be internally maintained in CFD solvers. As long as extracted CFD datasets are readable by ParaView, various data formats can be considered in the data processing software concerning data size, processing performance and quality. *Server-script* runs batch and bash scripts together with dedicated file handling operations to command executions in a row.

In order to automate the execution of modules in OpenFOAM, *Allrun* bash script was prepared to run each module in a user-defined fashion. Since the source code is not manipulated, no compilation is required in the system. OpenFOAM gives an output of each time-step separately in native format. A ParaView post-processing state was generated to automate the whole post-processing and data extractions tasks in the routine of OpenFOAM.

Unlike OpenFOAM, COMSOL only gives an MPH output file which cannot be directly processed in ParaView. Therefore, an extract-based data processing approach should start from the CFD solver. COMSOL has a post-processing module that can extract visual CFD data in VTU formats as a visualization toolkit (VTK) asset, thus enabling data processing in ParaView. All required orders should be set in the solver to extract and process necessary data through the automation routine. Automation was maintained with a JAVA file that is exported from COMSOL after completing a baseline simulation case. The JAVA file should be compiled with a suitable version of the JAVA software development

toolkit (SDK) in the server. A CLASS file was automatically created after the compilation. The *server-script* then requests a new COMSOL project with the CLASS file and executes orders from batch without GUI. It should be noted that COMSOL is commercial software and comes with several prerequisites to protect data-in-use. All preferences in settings must be switched to authorizing external activities and interaction with changes while preparing the case files. The *server-script* should be accompanied by *Allrun* batch script on Windows to command COMSOL executions. Moreover, we utilized the compact history feature in COMSOL through which redundant steps in the development were discarded to create a JAVA file giving all steps straightforwardly.

4.3.3 Data processing software: integration of CFD data with game engine

The data generated with CFD post-processors is not compatible with the game engine, hence, it is a must to further process CFD data to data formats that are readable by cross-platform environments. A data processing methodology was previously published to integrate CFD data with game engines [168]. The study proposed an extract-based data processing strategy upon open-source, lightweight, modular and automated elements in the processing pipeline with software written in Python. It provides a remote data processing approach that makes any user device employable regardless of its computational power. A widened investigation was also performed among the most commonly used data formats to integrate CFD data with Unity. The methodology additionally presented a module to tune processing parameters based on data processing speed, size and quality. In the present study, we applied the same methodology to integrate, optimize and automate the data processing in the two-way coupling.

4.3.4 Data in game engine and user application

A remote connection between data and user application is the backbone of the automated two-way coupling. Once a user application is built in Unity with default settings, it behaves as standalone offline software. The content in the application is inherently static without any remote interaction. Unity can be used to configure a CDN maintaining a remote connection between servers and clients. This way data can be streamed in the user application in runtime by avoiding default standalone built-in features. To develop a CDN with Unity, the user application should be linked to a server with a static connection during the cross-platform built-in. The following sections scrutinize the utility of features in Unity to generate a CDN in the client-server network.

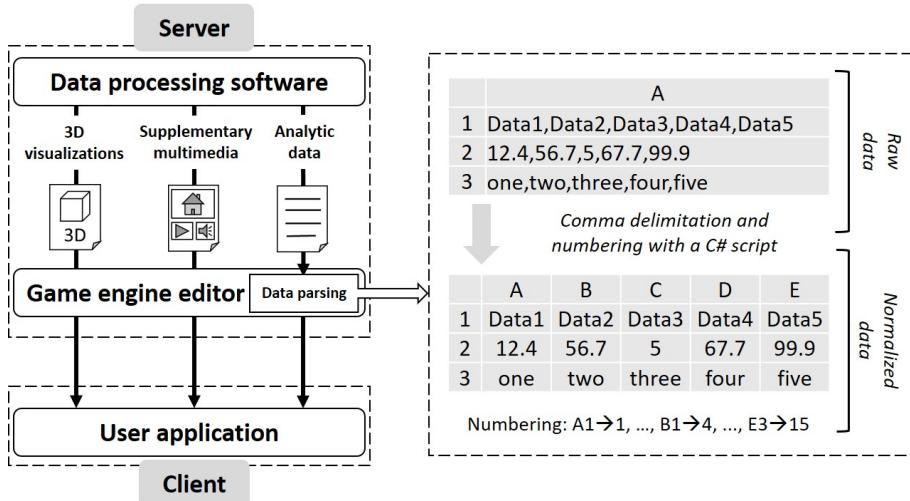


Figure 4.5: An example of data normalization in Unity.

Data normalization and representation

CFD visualizations, supplementary multimedia and analytic data are three data types processed and subsequently integrated into Unity. While the first two can directly be utilized in Unity after the data processing software, the latter needs internal handling as shown in Fig. 4.5. Text-based files generally consist of raw data, which means that the information in a file should be split into parcels to be correctly interpreted. A simple data parsing algorithm with `getText.cs` script in Unity is applied to transform data in a readable type to retrieve and stream in user applications. Without data parsing, Unity displays all information simultaneously. On the whole, the parsing algorithm creates a grid of parcels, and numbers each parcel with a specific number to easily locate and stream data. Any changes in the text file are automatically updated, parceled and streamed in runtime.

Each simulation data requires a GameObject to be stored and represented in the user applications. A GameObject in Unity is a component that may contain varying information to create functional objects. For instance, a 3D simulation data is a GameObject comprising location in the spatial domain, 3D geometry, texture and datasets. Representation of simulation data, as in the form of GameObjects, should be manually settled only the first time. The information is automatically updated in the relevant GameObject if it is linked to the CDN.

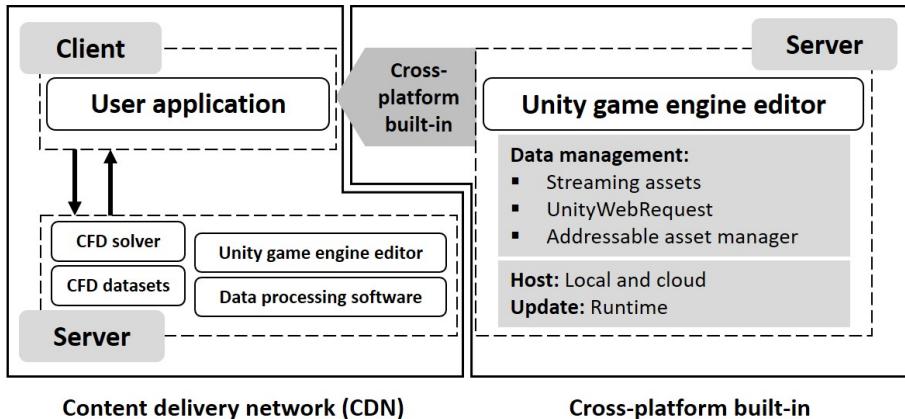


Figure 4.6: Content delivery network and cross-platform built-in in the client-server network.

Cross-platform built-in and content delivery network

Unity generates user applications with data stored in the project's asset directory during the built-in. No connection is maintained between data and user application by default. This results in standalone user applications that should be rebuilt with the game engine for any intended updates [174]. A dynamic connection between data and user application is one of the pillars of two-way coupling. Unity comprises well-oriented data management tools that are fundamental to host, manage and stream data remotely without any rebuild required. Fig. 4.6 illustrates an overview of the tools that were implemented in our work to develop a CDN in the client-server network.

Data management in Unity can typically be classified as file-based, unity package, asset bundle manager, and addressable asset manager. The latter is the most advanced type and brings miscellaneous options to handle data in Unity. It manages memory in runtime, groups assets in catalogs, makes connections to load assets from remote servers, and bundles assets efficiently concerning data size, processing speed and quality. In this study, the connection between data and user application was mainly built with the addressable asset manager in Unity editor. Addressable options were activated for target GameObjects to build addressable content that can be renewed from a remote server. On occasion, streaming assets with UnityWebRequest were also considered to be nearly static, seldom, updated and simpler dataflow. Both approaches provide a modular system for composing HTTP requests and handling HTTP responses

in runtime between client and server.

4.3.5 Dynamic post-processing in the client

Post-processing of CFD simulation data is a heavily interactive and iterative step taken manually by a competent analyst to present meaningful data. Once an optimal state is reached, the post-processing turns into a repetitive task that can be automated with a post-processing state file in the two-way coupling. Besides, additional interactive features in the user application may help non-expert users to increase comprehension of simulation data, as well as to provide flexible but restricted data exploration. In doing so we developed a dynamic post-processing data pipeline providing a connection between the client and data processing software in the server, as shown in Fig. 4.1.

Literature mainly demonstrated workflows to reprocess simulation data in the user applications. First, the native CFD data is processed in a CFD post-processor and results are exported in a dedicated format. Following, the exported file is transformed through the hardcoded methodology to integrate data with regard to the cross-platform. Finally, the file is exported in the cross-platform environment to reproduce data in the user application. This approach generally needs a lot of development work in case a change is intended to utilize another post-processing feature. Also, a suitable user device should be employed to handle comparable heavy data processing.

Our methodology differs from that in the literature. We do adhere to extract-based and modular features. Similar to the first connection in the client-server network, a case file-based dataflow was targeted, thus enabling a modular entity to maintain dataflow. The case file of the post-processing was embedded in the user application. Having updated the case file, the *network-script* sends the file to the server, in which the post-processing is performed, and streamed back to the client subsequently. A Python API-based implementation was achieved with open-source inter-connected modules of ParaView, VTK and Python. In essence, ParaView and VTK are widely used for advanced post-processing tools. Within the state file-based connection, any feature of these tools can be integrated into the user application through VTK classes, including case-specific post-processing methods. Basic post-processing entities, such as slicing, clipping, animating and color map labeling, were initially implemented in the user environment. We also built a simple animator to visualize transient simulation results in sequence. The user can play all time-steps, move between frames and create loops, as in a videocassette recorder.

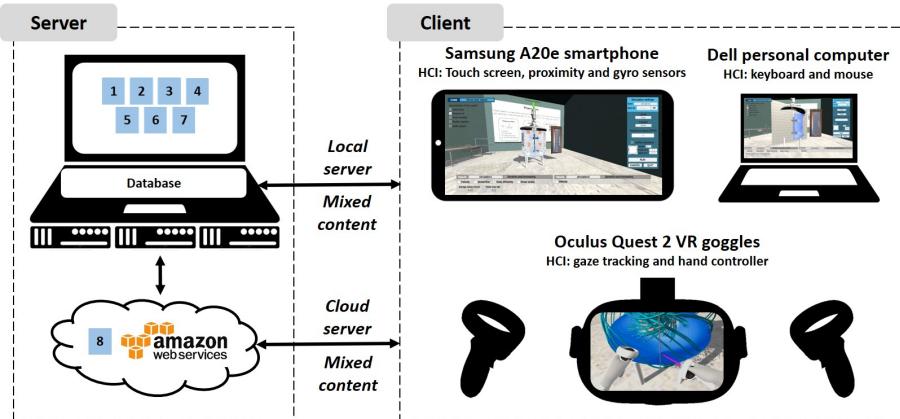


Figure 4.7: Implementation of the client-server network and connected user applications with relevant HCI components.

4.3.6 Case study

A case study was performed to assess two-way connection with user applications. A client-server network was maintained using heterogeneous modules to easily access different resources. A Dell laptop with Intel(R) Core(TM) i7-8850U CPU 2.6GHz - 32 GB with Windows 10 and Ubuntu 14 OS was set up to run modules in the client-server network. Fig. 4.7 shows the implementation of the client-server network.

Both OpenFOAM v6 and COMSOL v5.6 were integrated into the user environment. CFD simulations were carried out to analyze a stirred tank reactor investigating a liquid mixing process. OpenFOAM simulation was performed to optimize baffle plate arrangement in the tank by customizing mixerVessel2D tutorial. A k-epsilon turbulence model was utilized to model fluid flow with 2D and steady-state arrangements. A computational grid was structured with 76800 quadrilateral cells. Likewise, simulations in COMSOL were calculated to compare different impeller characteristics utilizing Mixer application from COMSOL application gallery. A 3D transient simulation of the mixing tank was derived to assess mixing characteristics with radial and axial impellers. Fluid flow was modeled with the algebraic yPlus turbulence model and 103197 tetrahedron cells were processed in the computational grid.

User applications and CDN were developed with Unity game engine 2019.2.18f1. We maintained the connection using one local on the laptop and one cloud-based host from Amazon Web Service (AWS). Three executable user applications were

developed, a mobile application for Samsung Galaxy A20e 32 GB with Android 10, a desktop application for the laptop with Windows 10, and a VR application for Oculus Quest 2 64 go. A walkthrough video of the VR experience is available in the Supplementary information for Chapter 4.

4.4 Results and discussion

4.4.1 Overall system performance

The two-way coupling consists of several connected modules in the client-server network. Data is processed in the server and then streamed in the user application. It was revealed that the entire coupling can be managed with modular API-based connections. Fig. 4.8 shows the overall system performance of two-way coupling through the client-server network. The system performance was obtained as the average of 10 repetitions with a 1.4% maximum error rate of the processing time. Each automated CFD routine was ordered to process a package of simulation data with the same size consisting of a 3D model, image and analytic data. The total processing time between the client's request and the server's response takes less than half a minute, excluding calculations in CFD solvers. The results indicate the importance of handling all data processing work in the server instead of in the user devices. Only the lightweight, mobile-friendly data is circulated in the client-server network. In both cases, output data sizes were reduced from 60 MB to 3 MB thanks to the extract-based data processing approach, thereby requiring 20 times less memory in the end-user device.

The total processing time in OpenFOAM covers CFD data post-processing since ParaView can directly be applied to the native CFD datasets. In contrast, COMSOL performs post-processing inside the software. Visual extracts are then processed with the data processing software to integrate data into Unity. In addition, COMSOL requires a compilation before running a new simulation from the JAVA file. Therefore, automation of COMSOL tends to take longer than that of OpenFOAM, as shown in Fig. 4.8. If the time spent during compilation is counted as a part of the automated routine, both CFD solvers approximately take 13 seconds to maintain a two-way connection. Table 4.1 presents a chart with details of connections in the two-way coupling cases. Employing more powerful hardware in the server can further lower the processing time spent in each module. The system collects extract-based simulation results to develop a database in the meantime. If the request of the user is previously calculated and stored in a database in the server, in only a few seconds the user receives a response and streams data in the application. Scenes from mobile, desktop and VR applications can be seen in Fig. 4.11 and Fig. 4.12, respectively.

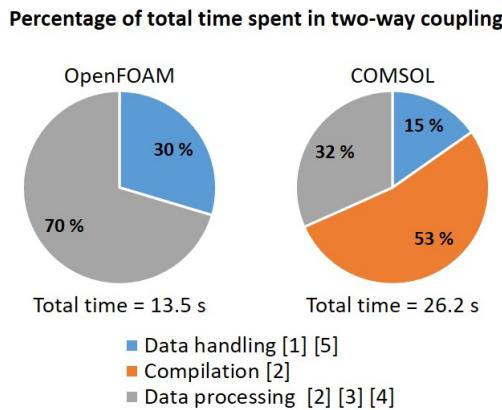


Figure 4.8: Overall system performance of the connection and comparison among CFD solvers, percentage of total time spent in two-way coupling.

Inevitably, interactive CFD simulations may take far longer time periods and a higher number of post-processing steps than what has been demonstrated in the implementation. It should be noted that educational simulations can be carried out for simplified but still accurate cases, especially targeting abstract examples. This may sufficiently serve CFD non-experts to learn the fundamentals of technical content and the concept of CFD simulations. As well, concerning generic but case-specific applications, reduced-order models (ROM) can be considered in the pipeline, which is becoming popular in the context of digital twins.

Table 4.2: The blueprint of automated two-way coupling with details on the system performance.

Connection	Parameters	User input [1]	Client to server [1]	Compile [2]	Automated CFD solver [2]	Data processing [3, 4]	Server to client [5]	Streaming in client [5]
OpenFOAM	Data type	OpenFOAM case	OpenFOAM case	-	OpenFOAM case	Mixed data	Mixed data	Mixed data
	Input data	text	C code	-	C code	C code	FBX; PNG; CSV	FBX; PNG; CSV
	Output data	C code	C code	-	C code	FBX; PNG; CSV	FBX; PNG; CSV	FBX; PNG; CSV
Processing time (s)		1	1	-	268	9.5	1	1
Output data size (MB)		0.004	0.004	-	60	3	3	3
Handler		client	network-script	-	server-script	server-script	network-script	client
COMSOL	Data type	COMSOL case	COMSOL case	COMSOL case	COMSOL case	Mixed data	Mixed data	Mixed data
	Input data	text	JAVA code	JAVA code	JAVA CLASS	VTU	FBX; PNG; CSV	FBX; PNG; CSV
	Output data	JAVA code	JAVA code	JAVA CLASS	MPH; VTU; PNG; CSV	FBX	FBX; PNG; CSV	FBX; PNG; CSV
Processing time (s)		1	1	13.9	2487 + 6 (post-process)	2.3	1	1
Output data size (MB)		0.121	0.121	0.085	60	3	3	3
Handler		client	network-script	server-script	server-script	server-script	network-script	client

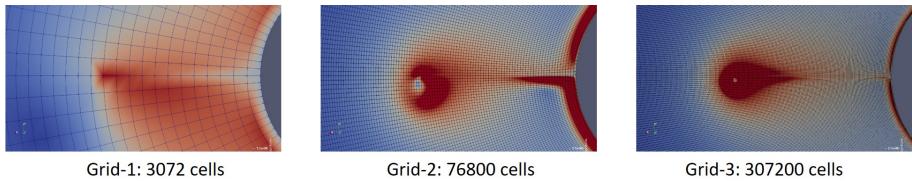


Figure 4.9: Number of grid elements used in the comparison.

Table 4.3: The effect of CFD model scale on tessellated data size.

Parameter	Grid-1	Grid-2	Grid-3
Number of cells	3072	76800	307200
OpenFOAM file size (kB)	941	23100	95800
Data processing time (s)	2.55	10.05	33
FBX tessellated data size (kB)	3271	3271	3271

4.4.2 Effect of CFD model scale on data processing quality

In a traditional CFD data visualization pipeline, the visual data is recalculated each time from data points encoded in a native format. In contrast, in the present study, a data processing software is employed to integrate CFD visual data with Unity by transforming native CFD data to tessellated data formats. The processing creates textures and tessellated geometry models from native CFD data, resulting in drastically reduced data size and processing time. A user device can readily handle and stream processed data without any heavy calculation required. A comparative study was carried out to probe further on the effect of the total number of grid elements in tessellated data size. Fig. 4.9 illustrates three different computational grid structures with varying cell numbers. It was observed that total numbers of elements in a grid do not show an influence on tessellated data size (Table 4.3).

Another concern over the integration of CFD visual data with tessellated formats was reduced data quality on screen and resolution. To assess this, we compared the processing of ParaView in VTU format to tessellated data in FBX as shown in Fig. 4.10. The comparison highlighted that the grid structure utilized in the simulation is kept the same or tessellated during the data processing as long as triangulation is performed in the post-processor. A texture is created based on data points on the grid structure, thereby keeping the resolution equal. This concurs well with a recent study on the data quality of tessellated formats to integrate simulation data with Unity [171]. Resolution of graphics should be

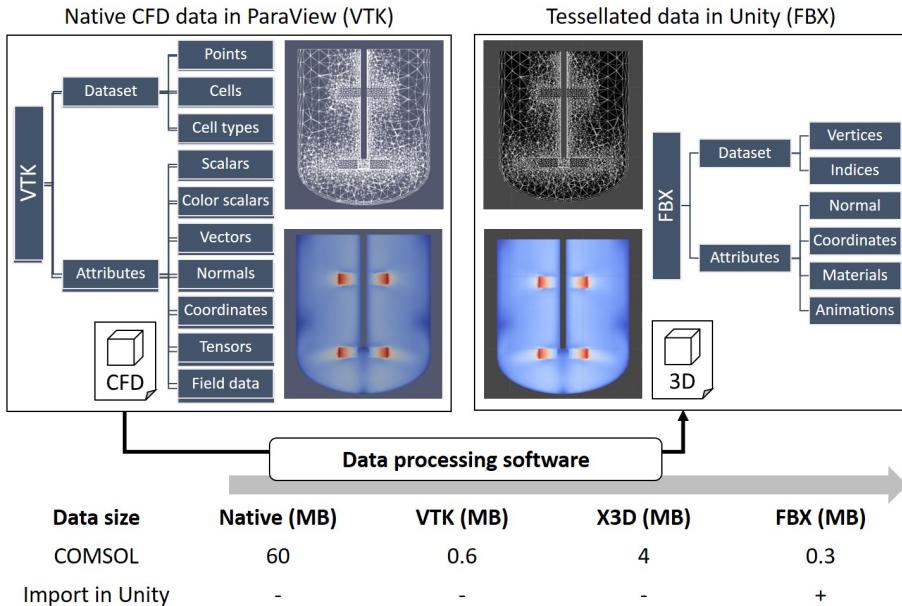


Figure 4.10: Data resolution throughout processing and integration of visual CFD data into Unity.

adjusted in Unity with regard to the user hardware employed such as texture resolution from render scale and anti-aliasing filter.

4.4.3 Data recovery in COMSOL

Data consistency and transient processing

Preliminary data extraction from COMSOL was previously mentioned in order to read data with ParaView. It was revealed that the extracts created in the design workflow should be kept in the working directory of COMSOL as a reference for the automated cases. Otherwise, even if the JAVA file processes a command to extract data during the processing, the software gives no input without references. Furthermore, it was observed that transient VTU extracts of COMSOL cannot be simultaneously imported in ParaView. The transient data should be piled with a PVD merger created with ParaView.

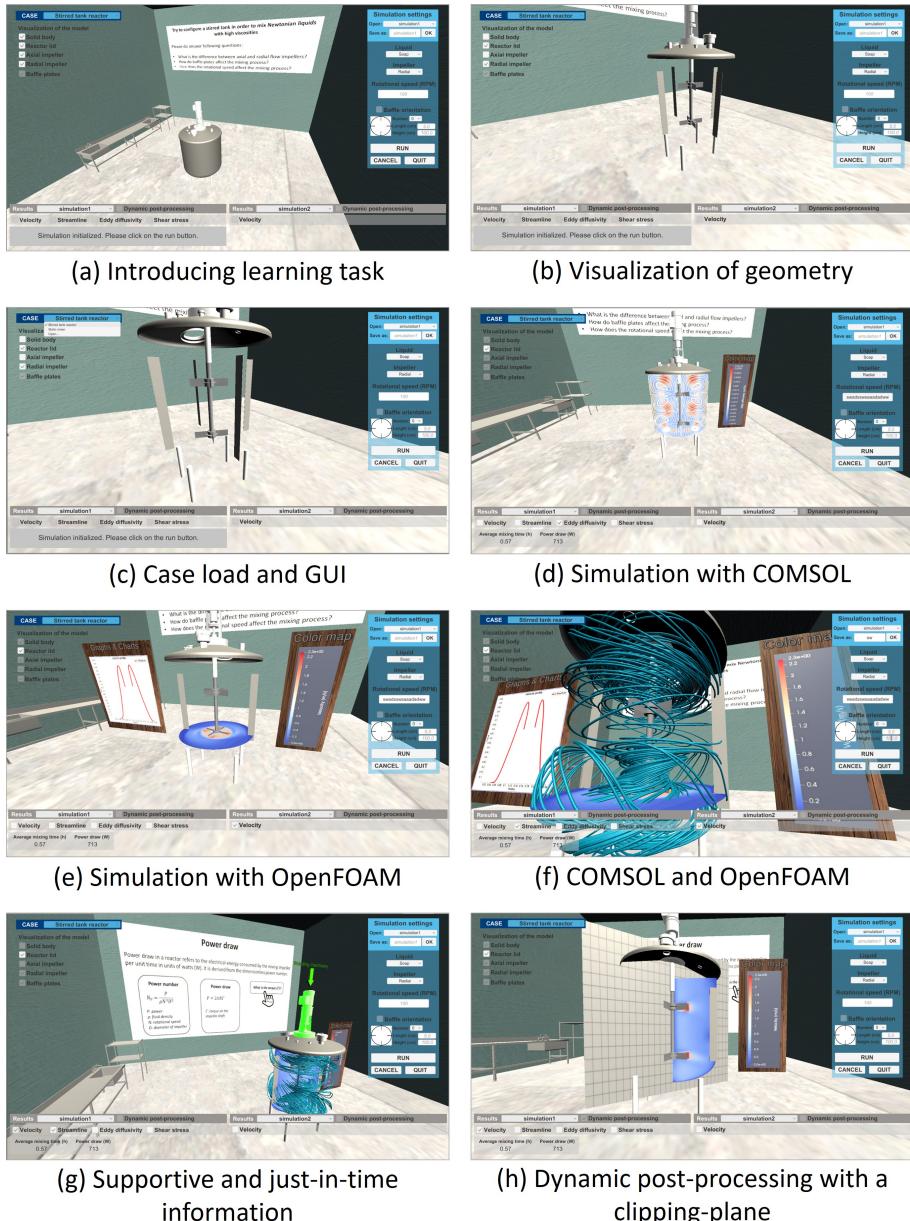


Figure 4.11: Scenes from desktop and mobile user applications.

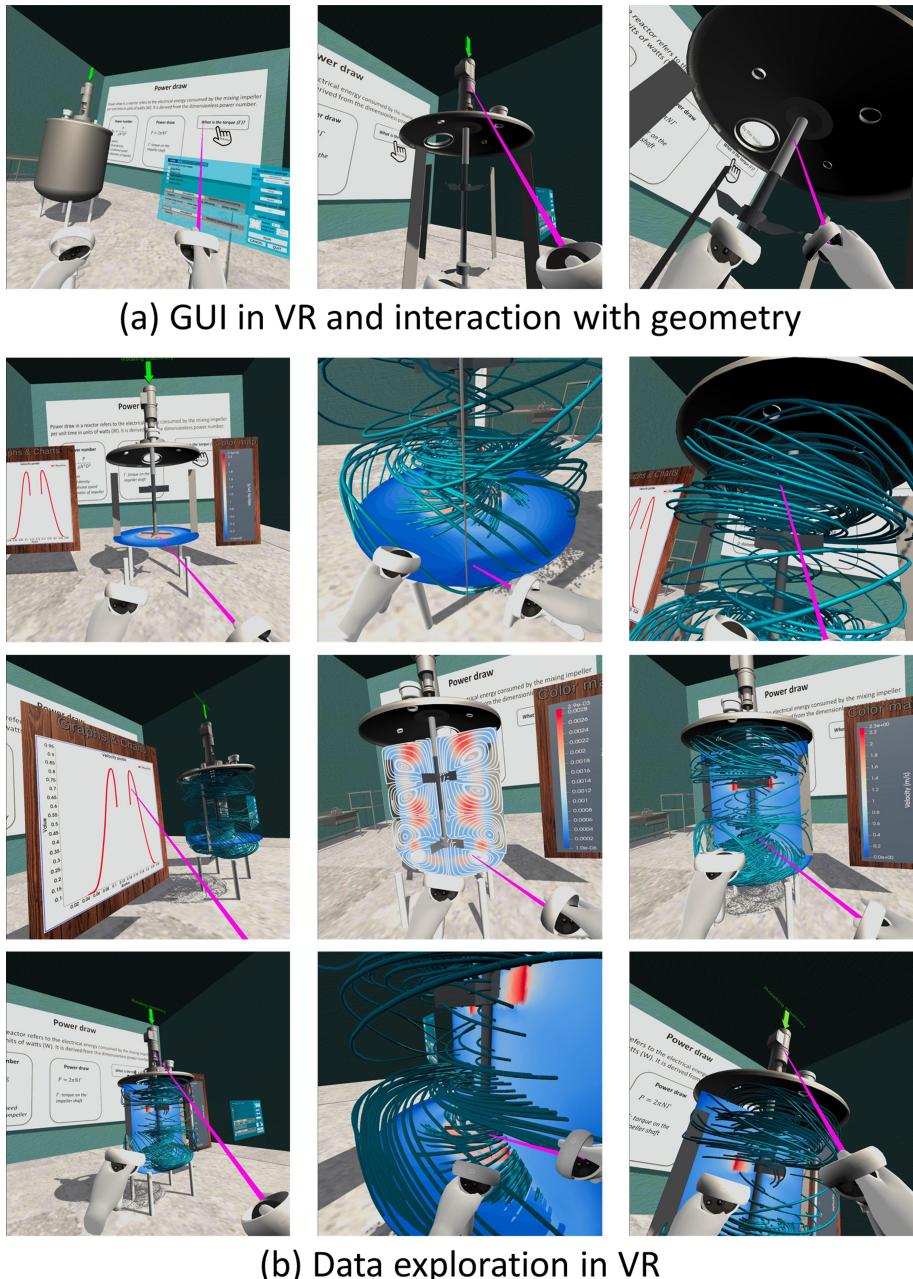


Figure 4.12: Scenes from the user application in Oculus Quest 2 VR headsets with hand controllers.

Processing streamline data

Streamline is one of the most used post-processing methods to visualize CFD data. It is formed from curves and splines derived from each cell point. A geometric extrusion is generally applied to extrude 3D structures in tube formats. COMSOL saves native CFD data in MPH format, which cannot be imported in ParaView without any preliminary processing in the software. To integrate the visual CFD data produced with COMSOL in Unity, COMSOL can export CFD visual extract in VTU format as an asset of VTK legacy, thus enabling data processing with ParaView. It was observed that VTU encodes only simulation data rather than geometric features, hence, the format does exclude all geometric features while extracting data from COMSOL, for instance, extrusion of streamline tubes from splines. An analysis was carried out to overcome this issue. The analysis revealed that Blender can extrude tube forms from bevel curves which would be an alternative way to recover streamline data in VTU format as shown in Fig. 4.13. Data processing software, presented in Section 3, comprises Blender as an intermediate data processor transforming CFD native data to tessellated formats. Therefore, data recovery can be directly performed in the data processing module by adding the if statement conveyed with Listing 1.

Listing 4.1: Extrusion of streamline data in VTU data format with Blender using bevel modifier.

```
scene = bpy.context.scene
scene.layers = [True] * 20 # Show all layers
for obj in scene.objects:
    if obj.type == 'CURVE':
        scene.objects.active = obj
        bpy.ops.object.mode_set(mode='EDIT')
        bpy.context.object.data.bevel_depth = 0.02
        bpy.context.object.data.bevel_resolution = 2
        bpy.context.object.data.fill_mode = 'FULL'
        bpy.ops.object.mode_set(mode='OBJECT')
```

Moreover, streamlines in the 3D tube format do result in large data sizes and processing times. Extrusion of streamlines with Blender can reduce data size and processing time by tuning the depth and resolution of 3D tubes. We carried out a study to elaborate on our tuning approach as shown in Table 4.4. Different data formats and processing pipelines were compared based on extrusions in ParaView and Blender. FBX opted for the final tessellated format. Interestingly, extrusion in ParaView drastically increased metadata produced

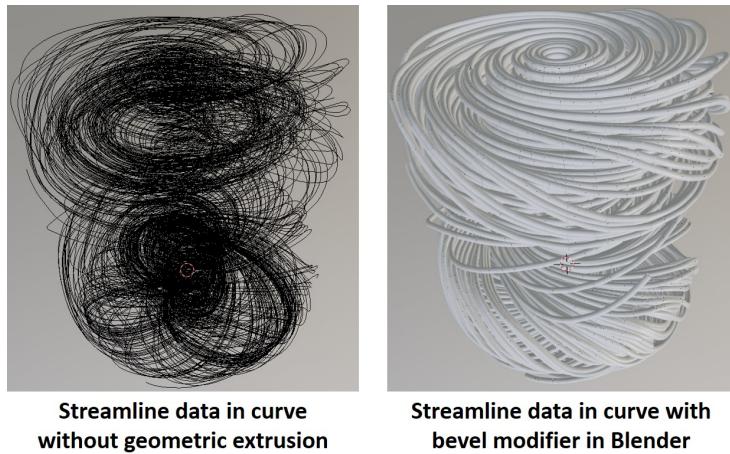


Figure 4.13: Streamline data recuperation from VTU file; without geometric extrusion (left); bevel modifier in Blender (right).

along the process. Even though it did not affect the size of the final data format FBX, the process results in large metadata temporarily being kept in the server. Extrusion of streamline in Blender (# 1, # 2 and # 3) requires lesser meta-data size and processing time than other workflows. This result confirms the usefulness of Blender in data recovery. The same processing methodology can be applied to tune point clouds and vector-based processing. In addition, data processing workflows of GTLF, OBJ and PLY formats without extrusion in ParaView failed to export simulation data from ParaView to Blender.

Table 4.4: Streamline data processing pipeline and comparison among workflows.

Work-flow	ParaView				Blender			
	Size (MB)	Extrusion (mm)	Time (s)	Export format	Size (MB)	Extrusion (mm)	Time (s)	Export format
#1	15.3	no	0.5	X3D	21.79	r=12	5.93	FBX
#2	15.3	no	0.5	X3D	22.07	r=5	6	FBX
#3	15.3	no	0.5	X3D	16.6	r=5	4.6	FBX
#4	17.8	r=12	0.3	GLTF	43	no	6	FBX
#5	90	r=12	2.7	OBJ	21	no	104.8	FBX
#6	152	r=5	4.86	X3D	21.74	no	19.7	FBX
#7	152	r=12	4.93	X3D	21.92	no	19.6	FBX

Table 4.5: System performance of dynamic post-processing in the client.

Connection	Dynamic processing approach	Client-server network	Total processing time (s)
OpenFOAM to Unity	#1 Already processed and stored in the database	6-5	5.5
	#2 Processing required		
COMSOL to Unity	#1 Already processed and stored in the database	6-5	3.9
	#2 Processing required (from VTU)		
	#3 Processing required (from MPH)	1-2-3-4-5	48

4.4.4 Dynamic post-processing

We developed a connection for dynamic post-processing in the user device as shown in Fig. 4.11*h*. Giving a flexible, dynamic but thoroughly constrained post-processing environment can assist non-expert users to grasp knowledge and deeper data exploration. Dynamic post-processing performances of OpenFOAM and COMSOL by means of methodology and data processing time are shown in Table 4.5. If the relevant post-processing is available in the database, marked with # 1 in Table 4.5, the system only takes a couple of seconds to stream data in the user application.

The dynamic post-processing in OpenFOAM is carried out with either native CFD data or data extracts in VTM format. User input from the client is processed to the state file and then sent to the server. Developers can create interactive elements for any intended parameters with ParaView API through the state file. This technique shows a fast and robust way to post-process data with user interference. Since Native OpenFOAM data is directly processed with ParaView, any specific need can be embedded into the game engine with a state file. This provides a wide range of utilities to process data thoroughly including slicing, clipping, animating, as well as any case-specific post-processing with VTK components such as vtkFilters. The same approach can be utilized for available VTU extracts from COMSOL, which is highlighted with # 2 in Table 4.5. Data is rapidly processed and subsequently streamed in the user application without including COMSOL and MPH files in the pipeline.

The technique requires a complementary workflow for COMSOL in case the intended dynamics post-processing does not have a VTU extract available in the database. In this approach, user input should be directly processed by COMSOL to extract relevant parts of the data. As mentioned previously, automation

of COMSOL was maintained with the JAVA file in the client-server network. The software executes each line in the file subsequently from the ground up including pre-processing, calculations, post-processing and data extraction. No matter what is processed in the JAVA file, the procedure repeats the entire cycle from the first line. To prevail over this redundant process in dynamic post-processing, we proposed an alternative technique. In contrast to the JAVA API file-based connection, the system directly executes the user input with the *server-script* using the COMSOL MPH file from the batch. The workflow, therefore, can bypass steps until the post-processing. The *server-script* finds relevant native COMSOL data in MPH format from the database and processes the intended parameters with *edit* through the command given in Listing 2.

Listing 4.2: An example of the command for running dynamic post-processing with COMSOL from batch.

```
"C:\...\comsol.exe"  
-edit C:\...\mixing3d.mph  
-Dcs.canvascolor=150,0,0,0,150,0
```

Alternatively, COMSOL has a *method* feature to keep on recording actions taken by analysts in the software. Creating a custom method in COMSOL automates user-defined settings that can be executed later on calculation from batch without GUI interventions. The *server-script* can perform the execution from the following command line added in the batch file as in Listing 3.

Listing 4.3: An example of the command for running dynamic post-processing with a method created in COMSOL from batch.

```
"C:\...\comsolbatch.exe"  
-inputfile C:\...\mixing3d.mph  
-methodcall methodcall1
```

The main pitfall of dynamic post-processing with COMSOL from an MPH file is the processing time which takes more than half a minute, comparably higher than other processing discussed above. Another way for time-consuming dynamics post-processing techniques is to extract slices in sequence and keep them in the server with VTU format, therefore, the network does not need to run COMSOL. Since slices are 2D or iso-surfaces, not too much memory is allocated in the database.

4.4.5 Asset management in Unity to create a content delivery network

A CDN was generated to remotely update simulation results in the user applications. A built-in is only one-time required in Unity to develop a user application with CDN settings. Both streaming assets with UnityWebRequest and addressable asset manager were utilized to make connections for CDN within Unity. Either free or paid cloud store facilities can be implemented in CDN as long as a static URL is provided for streaming assets and addressable asset manager. In the present work, we allocated a cloud server from Amazon Web Service (AWS) to host and distribute data in the client-server network. A local host was also created to experience how a personal computer can be transformed into a webserver instead of using the AWS system. Both servers were implemented into the CDN developed with Unity using streaming and addressable asset system as shown in Fig. 4.14.

Streaming assets with UnityWebRequest can create a remote connection for any game object in the game engine editor. It was found as useful due to the simpler workflow, a very short C# script generally provided by Unity. The connection should separately be maintained for each object in the digital environment. The method is incapable of managing multiple data in the client simultaneously.

Compared to the streaming assets, the addressable asset manager brings several advantages to build sustainable, long-lasting CDNs comprising several high-level operations to manage data and dataflow. The implementation revealed that addressable asset manager increases asset building and loading speeds. It also helps with runtime memory management in the user application. Category creation and labeling are important features that come with the management system to handle multiple data types. The system piles assets in bundles of 3D visuals, supplementary multimedia and analytic data for each simulation case. Not only GameObjects but also scenes in Unity can be remotely deployed within the addressable system. This feature facilitates developers to easily switch between entirely different simulation cases in the user application as shown in Fig. 4.11c.

Moreover, the addressable asset manager gives uncompressed, LZ4 and LZMA options to store assets with bundles comprising mixed data formats. A further assessment was carried out to understand the data encoding structure of the management system. An asset bundle from a particular simulation consisting of a 3D model, multimedia image and analytic data was utilized. The result showed that LZ4 and LZMA data compression methods can reduce asset bundle size 1.58 and 3.05 times, respectively, compared to the uncompressed format. In terms of data processing time, no significant difference was identified

between the uncompressed and LZ4 methods to process and stream data in the user application. However, LZMA resulted in some time delay during the decompression of the asset bundle.

These results offer compelling evidence for the addressable system, however, due care must be exercised to implement the addressable data manager in a two-way connection. The game engine should be employed as an intermediate data processor to build and manage asset bundles before streaming in the user application. This brings 5 s of data processing time in the game engine, labeled with connection 8 in the client-server network (Fig. 4.1). The bigger the total file size gets, the longer the data processing takes. Despite the additional processing work and developer expertise required to apply addressable asset manager, it considerably aids in developing long-lasting digital environments with advanced management features and robust connections, especially if mixed content is an essential trait.

The CDN adheres to a network to stream data in runtime from a remote server. Although it can automate dataflow and manage data in applications, it also requires the continued support of servers and complicated software development workflows. Overall, our assessment is that a blended use of streaming assets with UnityWebRequest and addressable asset manager serves best to promote optimal ways to develop CDN with Unity. Beyond education, training, and broad communication, engineering design and analysis would benefit from the cross-platform integrity of CFD simulations through the CDN in the client-server network. This might open gates for interoperable co-simulation environments as shown in Fig. 4.11f, as well as the incorporation of digital twins with interactive CFD simulations for fast prototyping. Our work demonstrated a promising practice on the automation and management of CFD simulations in multiplatform environments (Fig. 4.11 and Fig. 4.12).

4.4.6 Data and database management in the client-server network

Both CFD solvers and Unity are structured with dedicated data management systems, hence, there is no need to control the internal circulation of data in these software. However, preliminary findings showed that the data in the two-way coupling should be handled with an external system with sub-entities due to strictly different data types in use. We proposed two distinctive containers under the database that are set in the server to manage extracts and CFD data as shown in Fig. 4.14.

The extract database is driven with server modules to operate the data streamed

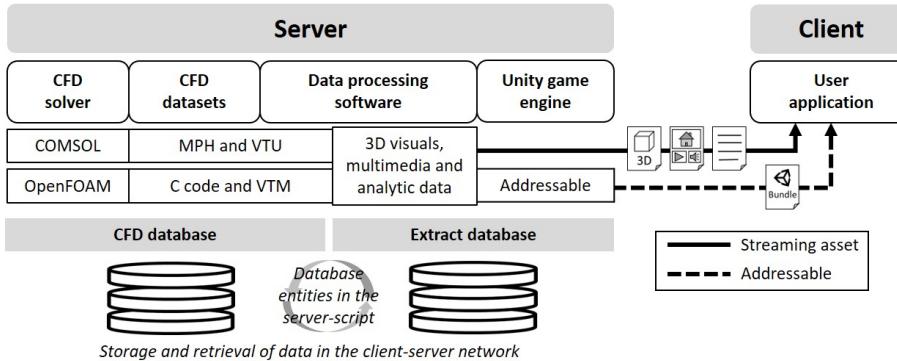


Figure 4.14: Automated two-way coupling with distinctive databases, streaming assets and addressable workflows to maintain remote connection in the client-server network.

in the client. Here multiple data formats, so-called mixed content, are dealt with as briefly explained in the previous sections. In general, extracts are kept as they are without any management, except documenting a particular simulation data in the same directory. Notably, a data management system dedicated to mixed content can provide a robust, long-lasting network to circulate simulation data between client and server. It was revealed that Unity provides an *addressable data management tool* to store, compress, retrieve and categorize the mixed content utilized in the user application through CDN. An analysis of the utility of the tool was elaborated in the previous sections.

The CFD database is utilized for storing and retrieving CFD data from multiple solvers. The results indicated that COMSOL encodes and saves entire simulation data in MPH format, hence, keeping only MPH files in the database is adequate for managing simulation software in a two-way connection. Additionally, VTK outputs can be hosted in the database if a dynamic post-processing feature is entailed in the workflow.

On the other hand, OpenFOAM keeps the case file apart from the data and outputs each time step in a separate directory. A study previously investigated the interoperability of different data models to store and retrieve OpenFOAM simulation data. The study suggested that the VTM data model, among several other models supported by ParaView, could be an optimal choice to store and retrieve OpenFOAM data for multiplatform utilities [168]. Our further examinations in this study revealed that data compressing models LZMA, LZib and LZ4 in ParaView enable a considerable reduction in data size while keeping the processing time almost identical to VTM without compressing method.

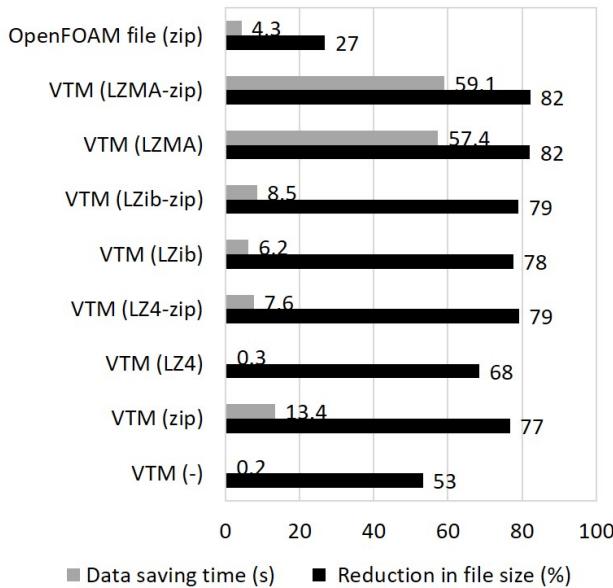


Figure 4.15: Assessment on the VTM model to store and retrieve OpenFOAM simulation data.

VTM with LZ4 performed the optimal analytics with a 68% reduction in data size and 0.3 s of processing time. A detailed comparison can be seen in Fig. 4.15. This method reduces the data size by orders of magnitude in a considerable period of time. In this study, we utilized VTM as a terminal data format to store and retrieve CFD datasets in the two-way coupling.

All database relevant jobs are executed with dedicated sub-entities in the *server-script*. Metadata produced along the coupling are temporarily kept until the target data is obtained. Data in the client is handled by the user application. The results of this study cannot be taken as evidence for all automated CFD simulation workflows. It is worth mentioning that several data formats can interchangeably be considered based on import and export features of the post-processing software. A preliminary assessment is a must to understand system database characteristics for multiplatform utilities. Although exploratory, this study may offer some insight into database structures. Two distinctive sub-entities might be necessary as long as extract-based data processing is applied in the integration of CFD data with Unity.

4.4.7 Some aspects of practical implementation

Necessary financial and human resources

Content creation, network and hardware are the fundamental pillars of two-way coupled systems. To develop such VR applications presented in the study, financial needs and competent human resources are required.

In order to minimize the financial needs, our work proposed multiple solutions to facilitate development workflows with open-source software. The workflow with OpenFOAM comprises only open-source utilities that can be freely integrated into the system without any copyright issues. In contrast, COMSOL is a commercial CFD solver, thereby requiring a license to produce CFD data. Nevertheless, the software comes with various supplementary resources to guide users to effortlessly perform CFD simulations within an advanced GUI. Neither user guides nor a built-in GUI is available for OpenFOAM. Developers should choose the convenient CFD software upon their expertise in CFD and programming. The rest of the software in two-way coupling are structured toward open-source utilities comprising well-documented resources provided within this study, as well as publicly available user guides. In addition, a powerful workstation is generally a necessity to perform CFD simulations and host the server in two-way coupling at the back end. Either university resources or in-house hardware can be allocated to set the system up. Also, cloud-based solutions may be a useful aid to deal with remote and computationally intensive systems. For offline and standalone applications, in which the CFD data is stored in the user hardware, there is no need for a server, thereby reducing the cost of hardware facilities. Furthermore, by means of end-user hardware, Oculus VR headsets cost around € 400 at the time this study was conducted in 2021. The VR market is dynamic and composed of several brands for which Unity can also build the same applications with cross-platform utilities. Developers may easily switch to other VR hardware considering financial and technical aspects. Alternatively, a smartphone version of the VR application with Google Cardboard might be a low-priced counterpart, as well as an accessible technology. It is plausible that smartphone-based solutions adversely limit the effect of the immersion as they lack peripheral devices and relevant HCI components.

A diversified human resource is imperative to set up VR applications with CFD simulations due to the interdisciplinary structure of the study. Collaborative work should be prompted between developers and practitioners to overcome design and operational challenges. Our work includes a development strategy with provided tools that can be replicated by volunteers. We tried to divert conventional workflows into modular, easy-to-implement and coding-free utilities. Notably, proven expertise in CFD and computer science can drastically diminish

the workload in the development. In addition, the design of educational digital environments should be critically examined with university lecturers to obtain the optimal user experience for targeted student groups. To sum up, it can be helpful to compose a project group of people with diversified competencies, which can smooth the way during the design and development phases. Initial user prototypes can be roughly made ready in a couple of weeks. Agile development cycles with preliminary user studies are also strongly recommended to tune the user experience in VR environments.

Insights on educational practices

CFD simulations can bring heuristic solutions for fluid flow and multiphysics problems that are difficult and costly to study with physical experiments. Chemical engineering comprises several abstract concepts that can be intuitively examined with CFD simulations. Integration of these simulations in user-friendly VR environments may help students perform virtual experiments while learning from meaningful simulation content. VR applications can also leverage cognitive skills with advanced HCI, whereas students' motivation can be augmented within user-friendly, fun and engaging environments. This may allow both students and lecturers to benefit from CFD simulations while making them accessible in the early stage of higher education. VR applications have a wide range of scalability blending advanced learning content, technology and pedagogy in a unique way. This can be helpful for lecturers to divert the user experience upon the needs of their target group from edutainment over stimulating academic interest to advanced visualizations. In addition, real-time feedback and data collection are other positive aspects of VR applications. Lecturers may exploit built-in assessments by keeping track of user actions in the VR application in the context of learning analytics.

Notably, VR applications can be blended with traditional lab courses being either complimentary or supplementary to physical experiments throughout content-wise rich educational practices. This may boost students' interaction with technical content whereas lecturers may touch upon challenging concepts that are not possible with current educational technologies. Interestingly, CFD simulations in the VR environment can be readily transformed into augmented reality (AR) applications [175]. This may enable embodied collaborative tasks that students can experience and take while physically being present in the laboratory. For instance, transport phenomena in microfluidics with an AR experience, as a complementary tool for a lab course, may leverage both cognitive and behavioral aspects of educational practices. For verified and validated simulation workflows, neither lecturers nor students have to know the operational aspects of CFD simulations at the back end. Our discussions are restricted

with supplementary and complementary utilization of such applications in lab courses through an act of balance that should be taken into account by lecturers. Replicating the entire lab experience with a virtual environment should be treated with utmost caution from a pedagogical point of view.

Inevitably, utilization of VR applications in education can be restricted - even avoided - because of the struggles both students and lecturers may face. From the lecturer's point of view, accessing the required amount of VR headsets for an entire classroom can be found financially challenging. In addition to this, the development, implementation, post-production and maintenance of such digital applications may increase the workload on lecturers. Therefore, a good way to avoid these hurdles is to compose a competent project group. Aside from technical concerns over the implementation of VR in classrooms, the impact of VR on students' health, so-called VR sicknesses, should be seriously taken into consideration by developers and practitioners. Both physical and cognitive harms may potentially arise from VR applications due to hardware- and software-induced deteriorations [176]. Students, who are vulnerable to VR environments, can develop negative side effects such as dizziness, disorientation, seizures, nausea and eye soreness. A meta-analysis on VR sicknesses revealed that the intensity of negative side effects is undeniably influenced by digital content, visual stimulation, locomotion, exposure times and user characteristics. Notably, the study illustrated the importance of simplified digital content and relatively low exposure times to tackle the negative implications of VR environments [177]. Lecturers should keep an eye on students to comprehend their experience and identify major inadequacies preventing them to adopt new technologies. Performing technology acceptance studies within the preliminary prototypes may hint at these drawbacks to be avoided in the early stages of implementations. Recent publications delegate both developers and practitioners to alleviate negative side effects and ensure health and safety standards in VR experiences [176, 177]. Furthermore, a desktop version of the VR application, such as a computer game, can be built in Unity in order to avoid grave aspects of virtual reality for vulnerable individuals. Though immersive features of VR are diminished in the desktop version, students and lecturers can still benefit from the user-friendly educational digital application with CFD simulations.

4.5 Conclusion

This study presents a versatile development methodology to implement interactive CFD simulations with cross-platform environments such as desktop and virtual reality applications. We developed a client-server network to maintain a two-way connection between CFD solvers and Unity, with promising

applicability to employ different client user devices without any computational demand. Essentially, the connection is a great enabler to develop technically advanced learning environments with CFD simulations, as well as digital authoring tools for educational technology developers. In addition, the implementation of multiple CFD solvers simultaneously in the game engine formed a co-simulation environment. Not only education but also engineering can benefit from the cross-platform integrity of CFD simulations, for example, communication of CFD simulations to broad engineering communities. Beyond, the system might be beneficial to settling up digital twins, if on-site connected interactive CFD simulations are added value for operational purposes.

Future studies will tackle technical content to be progressively incorporated from macro- to micro-mixing, thus providing a widened tool to teach transport phenomena. More functional environments will be deployed facilitating well-designed GUI and HCI components. Qualitative and quantitative user assessments will be performed to determine the effectiveness of the VR applications. We also intend to extend the user environment with inquiry- and game-based learning approaches to profit more from educational theories to motivate learners and trigger their curiosity.

Chapter 5

An immersive virtual reality learning environment with CFD simulations: Unveiling the Virtual Garage concept

The chapter is under review in a peer-reviewed journal: *Solmaz, S., Kester, L. and Van Gerven, T. An immersive virtual reality learning environment with CFD simulations: Unveiling the Virtual Garage concept.*

Author contributions: S. Solmaz conceived the research, performed the data analysis, interpreted the results and wrote the article. T. Van Gerven and L. Kester contributed with their guidance and expertise in this work.

Abstract Virtual reality has become a significant asset to diversify the existing toolkit supporting engineering education and training. The cognitive, affective and behavioral advantages of virtual reality (VR) can help lecturers reduce entry barriers to concepts that students struggle with. Computational fluid dynamics (CFD) simulations are imperative tools intensively utilized in the design and analysis of chemical engineering problems. Although CFD simulation tools can be directly applied in engineering education, they bring several challenges in the implementation and operation for both students and lecturers. In this study, we develop the *Virtual Garage* as a task-centered educational VR application with CFD simulations. The Virtual Garage is composed of a holistic immersive virtual reality experience to educate students with real-life engineering problems

solved by CFD simulation data. The prototype is tested by graduate students ($n=24$) assessing usability, user experience, task load and simulator sickness via standardized questionnaires together with self-reported metrics and a semi-structured interview. Results show that the Virtual Garage is well-received by participants. We identify features that can further leverage the quality of the VR experience with CFD simulations. Implications are incorporated throughout the study to provide practical guidance for developers and practitioners.

5.1 Introduction

Applied engineering deals with complex problems to provide efficient solutions for a sustainable world. As a result of this, engineering problems have become intricate and require interdisciplinary approaches to unveil novel solutions [11]. Teaching and communicating these problems may even get more complex since such practices require great effort to produce adequate content and materials. Policymakers have been actively addressing "digital education" to encourage a paradigm shift in education with high-quality, inclusive and sustainable tools [8].

Computational fluid dynamics (CFD) simulations are physics-based numerical tools heavily applied in engineering design and analysis to solve problems in a time cost effective fashion. CFD comprises not only hard skills but also soft and cognitive skills such as critical thinking, decision making, creative problem solving and time management, together with advanced spatial reasoning skills [12]. Therefore, the educational use of CFD simulations may be essential to prepare young students for real-life settings.

CFD simulation tools can be directly applied in engineering education. However, they bring several challenges in the implementation and operation for both students and lecturers. First, the educational use of CFD simulations may be challenging due to an expert-centric user experience in conventional simulation and post-processing environments. It requires complex skills to perform CFD simulations and interpret obtained results to make justifiable decisions. Second, learning in conventional simulation environments often happens via learning by doing on 2D desktop settings. Such environments do not comprise any assistance except help options relevant to the usability of the tool. Learning by doing is criticized by educational scientists and found less efficient than traditional instructions [76]. Third, CFD simulation data can be utilized in the existing educational context in the form of video clips and images. However, in such practices, students cannot directly interact with simulation data, thereby merely experiencing a passive participation. Finally, lecturers should provide

sufficient supportive information to help students understand the basics of the problems solved by CFD simulations, as well as design adequate instructions. All these can hinder the utilization of CFD simulations and simulation data in education in an effective and interactive manner.

The assistance of virtual reality in support of immersive learning has been a hot topic in engineering education. Immersive virtual reality learning environments may reduce the entry barrier to cognitively complex learning subjects [15]. These environments can positively trigger cognitive skills with advanced spatial interactions and easy-to-access technical content, as well as affective and behavioral aspects of learning such as motivating students to adopt new educational technologies [6]. This might open gates for user-friendly, high-quality complex learning environments assisted with CFD simulations.

Developing VR environments with physics-based high-fidelity engineering calculations can create value to facilitate high-quality immersive and interactive educational tools [19]. Likewise, visualization of CFD data in VR can enable a better interface than 2D screens to work with complex datasets in the context of scientific visualization [38]. Many researchers have investigated the integration of CFD simulation data in immersive technologies, mainly targeting technical challenges [112, 16, 168, 40]. Given the complexity of CFD workflow and methodology, immersive visualization of CFD simulations in VR itself is not sufficient for non-expert users such as engineering students. The learning environment should be adequately structured considering relevant components of instructional design. It also appeared that more research on evaluations of prototypes including human factors is essential to provide better applications and unlock the potential of these tools from students to policymakers [16, 17, 39, 40].

Little is known about the educational use of VR with CFD simulations and it is not clear what factors should be taken into account in the design, development and evaluation phases. In this study, we present the VR application *Virtual Garage* which is a holistic immersive virtual reality experience to educate students with a real-life engineering problem solved by CFD simulation data. Our ultimate goal is to obtain evidence that helps address these research gaps in support of developers and practitioners to design and evaluate their own immersive learning environments with CFD simulations.

5.1.1 Related work

Visualization of CFD data via immersive technologies

Previous studies have evaluated case-specific visualization settings with users from varying disciplines [178, 179, 180, 181, 105, 117, 118, 182, 183]. In another research, visualization of fluid flow in immersive environments was evaluated with a quantitative approach to understanding nonexperts' interaction and experience. A statistical analysis was also performed to test different hypotheses to pinpoint the significance between different design parameters [184]. In general, studies evaluated technical design features with a very limited number of participants. Occasionally, interviews are reported to validate and improve visualization features such as colors, visual representations and interaction with simulation data. Conclusions were drawn upon the features to make simulation data more intuitive and accessible for non-experts in AR and VR.

Likewise, a recent study investigated the effect of immersion in the visualization of blood flow in the vascular systems by comparing a 2D screen, a semi-immersive screen and a VR head-mounted display (HMD) [36]. Both qualitative and quantitative analyses were performed to evaluate users' performance and intuition. VR HMD was found innovative and supportive to build cognitive abilities to visualize simulation data and manipulate geometry for different simulation settings. Another work carried out a media comparison study between desktop and VR HMD. A subjective evaluation was made to assess accuracy, experience and graphics with 8 participants. It was indicated that VR can increase the likeliness of experience and graphics [40].

A growing body of literature has evaluated the visualization of CFD data in AR and VR. Neither instructional design nor assisting educational content is utilized in the digital applications. User assessments were fundamentally conducted through qualitative analysis to get more insight into the cognitive outcomes of the immersive visualization of CFD data. Quantitative methods and standardized tests were occasionally considered by researchers.

Educational use of CFD data in immersive learning

In recent years there has been limited interest in the development of learning experiences with instructions in immersive learning environments with CFD simulations. A preliminary attempt was to implement a VR application with CFD data in a master course [119]. According to the qualitative assessments, even though negative aspects of VR such as simulator sickness and cost were reported, students overall showed a positive attitude toward the immersive

experience. However, several key challenges - such as how to tackle downsides to make the implementation easier for students - remained unsettled. In another attempt, a VR environment with CFD simulations and instructions was developed to educate farmers and decision-makers in a greenhouse [37]. A preliminary qualitative analysis was carried out, through which several improvements were processed in the user experiences such as supportive and procedural information, and also the design of a tablet-shaped graphical user interface (GUI). The assessment was only superficially reported and not profoundly discussed. Surprisingly, only one study considered the utility of standardized tests in user assessments [185]. A usability study with the System Usability Scale (SUS) was carried out on the VR application to educate gas engineers on the potential gas leaking scenarios. However, no perspective was given on instructional design and other aspects relevant to immersive learning environments.

A recent set of studies investigated the learning effect of a VR application to teach the basics of fluid mechanics and CFD [29, 166]. A quantitative methodology is applied with self-reported metrics to measure understanding and learning, and compare it to conventional teaching. The study claimed that CFD simulations in educational VR positively affected learning and increased students' interest in the content. It was also useful to help students comprehend mathematical equations and spatial reasoning to work with complex CFD simulation data. Subjective metrics were mostly utilized, and no statistical analysis was performed to show significance.

Finally, despite not using immersive technologies, we found another study worthwhile reporting since it compares real-time interactive and non-interactive CFD simulations in a user-friendly learning environment for non-experts [186]. Both performance and user experience are statistically analyzed through self-reported quantitative metrics. The study indicated that interactive simulations were less demanding than non-interactive ones. Interactive simulations also encouraged users to explore more parameters. Despite this, the overall task load did not change between interactive and non-interactive simulations. In both cases, since participants were novices to fluid dynamics, challenges were observed in the interpretation of CFD results, such as understanding water flow from visually represented CFD data. This affirms the importance of instructional design in learning environments with CFD simulations.

Recently published reviews have provided a broad list of challenges that are dramatically impeding the adaptation of VR in engineering education. A summary of conveyed challenges is available in the Supplementary information for Chapter 5. On the whole, many attempts have been made to assess technical and human factors with user studies including usability, simulator sickness, self-reported scales and learning. Available literature mostly focused

on users' interaction with simulation data. Most of the studies very primitively reported on important metrics and did not adequately process and analyze research data. Studies were also performed with a very limited number of participants, who were not – in general – truly representative of the target audience. Some applications also directly concentrated on learning outcomes instead of evaluating the quality of the digital environment before measuring the learning. Hence, very little is still known about the importance of human factors in educational VR experiences with CFD simulations. No immersive learning experiences with CFD simulations have been encountered in the literature. Neither learning theories nor instructional design models have been reported by developers.

5.1.2 Objectives and significance

Recent evidence revealed that each VR experience has a unique user experience with regard to simulator sickness [187]. We can arguably relate this to other human factors in VR since every VR experience is composed of various custom design elements such as GUI, instructional design and digital content. An analogous approach has been suggested based on Maslow's hierarchy of needs to systematically evaluate VR experiences from the ground up [188]. A preliminary evaluation of human factors is key to unlocking the potential of immersive learning environments to detect underlying and hindering effects before focusing on learning outcomes.

In this study, we evaluated the effect of CFD simulations in an immersive learning environment using the Virtual Garage. It is composed of two subsequent modules, Module#1 and Module#2. The former is a procedural learning environment to teach interaction in VR and provide supportive information on content with relatively easy tasks to be completed by users. The latter is an assessment environment mainly comprising data interpretation, problem-solving and decision-making by using pre-computed CFD simulation data. Even though both modules cover several learning content and tasks, it would appear that it is worthwhile to evaluate the added-value of CFD simulations. We, therefore, analyzed usability, user experience, task load and simulator sickness by performing a pairwise comparison between the modules. The following research questions (RQ) are purposefully formulated:

- RQ1: How does system usability change between the modules?
- RQ2: Is there any significant difference in task load between the modules?
- RQ3: How does the content affect the user experience between the modules?

- RQ4: Is there any significant difference in simulator sickness between the modules?
- RQ5: Is there qualitative feedback that may help further interpret quantitative results?

5.2 The Virtual Garage concept: what matters?

The Virtual Garage is a task-centered educational application composed of a holistic immersive virtual reality experience to educate students through a real-life engineering problem solved with CFD simulation data. It is the first-ever learning concept blending virtual reality, instructional design and CFD simulations. It stems from the frameworks of Technological Pedagogical Content Knowledge (TPACK) [189] and Substitution, Augmentation, Modification and Redefinition (SAMR) [45]. Both frameworks give a theoretical foundation for the design and development of digital learning environments. Only making technology and content available for learners is not the best practice for immersive learning environments. Suitable pedagogical approaches, such as instructional design models, should be implemented to leverage the quality and value of the educational experience. The following subsections detail the applied methodologies which laid the foundation for the Virtual Garage concept.

5.2.1 Pedagogy: instructional design matters

CFD simulations in engineering design and analysis adopt an active learning approach where engineers actively manipulate design parameters and produce data. Simulation results are generally analyzed in a heavily interactive process with specialized post-processing software to extract meaningful data in support of decision-making. Working with CFD simulations can be a complicated procedure requiring both technical skills and competencies while covering the entire cognitive spectrum in the revised version of Bloom's taxonomy of learning [12]. The taxonomy is a prominent framework to effectively identify the learning outcomes. It also categorizes and classifies cognitive skills to reach the utmost complexity in the learning process [67, 66]. Hence, it is extremely demanding for engineering students to adequately perform and learn in simulation-driven learning environments. A learning environment with simulation data should be properly designed not only concerning data visualization but also supportive and procedural information to sufficiently guide and support learners to prevent cognitive overload. According to the Cognitive Load Theory, instructional design is an essential tool to develop learning experiences that the human brain appropriately manages [68].

A good instructional design should consider both cognitive load theory and multimedia learning principles, and accordingly adapt them to learners [70]. CFD data is inherently multimodal and composed of varying multimedia such as graphs, charts, numerical data, 2D colored contours and 3D volumetric data with colormaps. Therefore, in order to prevent cognitive overload, it is imperative to apply multimedia learning principles to effectively communicate CFD results with nonexperts. Among several instructional design models, the four-component instructional design (4C/ID) is being increasingly applied in learning environments for complex learning [68]. The 4C/ID model deals with a task-centered complex learning environment accompanied by real-life tasks while incorporating design principles in multimedia environments [75]. From this perspective, the 4C/ID model is a good fit to design active learning environments with CFD simulations and immersive technologies. Therefore, we meticulously adopted the 4C/ID model in order to conceptualize and design the Virtual Garage concept.

The 4C/ID model comprises four major components to evoke complex learning; learning task, supportive information, procedural information, and part-task practice. Learning tasks are whole-task experiences based on authentic real-life problems that are supported by supportive and procedural information. For example, in the Virtual Garage concept, the whole-task experiences are real-life chemical engineering problems to be solved by CFD simulations, in which the complexity is progressively increased by applying the sequential principle. The whole-task model in 4C/ID is an imperative aspect of complex learning to simultaneously integrate knowledge, skills and attitudes, as well as appropriate coordination of skills. Besides, supportive information is the theory of the learning content to provide non-routine aspects of the domain and task that learners can unconditionally reach. Likewise, procedural information is timely and organized instructions to help learners perform routine aspects during the learning task. In contrast to whole-task experiences, part-task practices are practice items to assist learners to gain a high level of automaticity in a particular aspect of complex learning. Each component in the 4C/ID model is customized with design principles to orient them with specific learning objectives. A broad spectrum of principles with explanations is available in the relevant design guideline [72]. Details on the implementation of the 4C/ID model in the Virtual Garage with the relevant components, principles and examples are available in the Supplementary information for Chapter 5.

Moreover, we also implement a number of gamification elements in the learning environment to further exploit cognitive and affective domains in the context of immersive learning. A roleplaying scenario is embedded to fortify the real-life experience and immersion [83]. In this case, users are treated as engineers who are collaborating with stakeholders to solve a problem with CFD in an

industrial case study. This may help increase immersion from a pedagogical point of view. In addition, gamification can increase students' engagement and positively affect emotions [83]. For that reason, we create gamified tasks to provide interactive and joyful experiences such as puzzle games to grab and correctly locate 3D components of a reactor in a puzzle.

Both formative and summative assessments are made throughout the learning experience. As an example of formative assessment, in Module#1 after a certain amount of supportive information students are asked to complete a puzzle by matching keywords to correctly formulate the objectives of the case study. Similar formative assessments are distributed in the modules. Also, we incorporate a summative assessment methodology based on time, errors, achievements and decisions in the entire application. Overall performance is scored based on an assessment rubric with intended learning outcomes. At the end of their experience, students can observe their performance to make self-evaluations using a learning analytics dashboard. They can also retrospectively move into Module#2 to reflect on their decision whilst comparing it to the correct answer. After the VR session, we schedule a dialogue with students to let them reflect on their experience, which may help to form a long-term memory as recently proposed by researchers [190].

5.2.2 Virtual reality: immersion and interaction matter

Immersion and interaction are primary features of VR leading to cognitive, affective and behavioral states of users [191]. In the Virtual Garage concept, we utilize VR to deliberately give a boost in these states. While the VR experience can be engaging, motivational or fun, it can also help develop spatial understanding and reasoning skills. This is well in line with our objectives in the development of the Virtual Garage concept. The Virtual Garage is purposefully designed for a 6 degree-of-freedom (DoF) VR experience to unlock the full potential of immersion and interaction in the virtual environment.

In terms of user experience, we targeted a holistic VR experience to provide a standalone learning module, such as learning nuggets in microlearning [192], longer than traditional ones but similarly focusing on a case-specific learning activity without any external intervention. In particular, a recent framework has classified VR experiences that vary throughout a continuum between atomistic and holistic experiences [14]. Researchers drew a distinction between atomic and holistic models in terms of user experiences. They claimed that holistic VR may enable higher hedonic quality, in contrast to higher pragmatic quality for atomistic VR [14]. This should be evaluated by applying relevant metrics and scales in user studies.

Interaction and immersion of VR should be cautiously designed to mitigate simulator sickness. In the field of VR, simulator sickness refers to any physical and mental symptoms affecting users' well-being either during or after the VR experience [193]. Literature has recently been bombarded with research on simulator sickness. Several guidelines are made available to lead developers to mitigate simulator sickness in custom VR experiences [193, 176, 177]. A number of significant design parameters were taken into account in the Virtual Garage concept as presented in the Supplementary information for Chapter 5.

5.2.3 CFD simulations: content matters

Choosing CFD content that makes sense for students is an important aspect of the immersive learning experience in the Virtual Garage concept. For example, "flow past an immersed object" is a widely utilized case study to train and practice learners in fluid mechanics and CFD. The content is simple, visual and very cheap to calculate. However, the content fails to resonate among learners to teach the methodology and application of CFD since students cannot relate the physical phenomenon to everyday engineering problems. Therefore, from our perspective, it is crucial to find a real-life example and embed simulation content in it, as well as relate the learning experience to the existing engineering curriculum. In the Supplementary information for Chapter 5, we list a series of CFD content to teach intensified processes in chemical engineering based on a content map structured by screening the relevant curriculum.

CFD data should be carefully processed to present meaningful visual and textual data. More accessible colormaps should be applied in visual representations such as batlow color scheme [194] considering color blindness and visually impaired users. Realistic rendering of assisting digital content such as geometry with relevant textures may be helpful. Multimedia learning and relevant principles should be substantiated in the design of the simulation environment.

5.2.4 Prototype: concept matters

The previous sections detailed design guidelines utilized in the conceptualization of the Virtual Garage. Fig. 5.1 illustrates a schematic of the Virtual Garage concept with applied pedagogical tools. The entire VR experience is divided into two subsequent sections, namely Module#1 and Module#2.

Module#1 is composed of VR training and theory sections. The former aims at teaching hand controllers in VR. The experience resembles a playground where users practice interactions throughout playful tasks. It includes only formative

assessments to be completed by users before proceeding with the actual learning content. The ultimate goal of VR training is to get users familiar with hand controllers and interactions in VR, thereby negating the effect of any cognitive load due to the use of technology. The latter is the section where the theory is presented with supportive information together with preliminary tasks to evaluate users throughout a formative assessment scheme. Users consume the content and complete playful tasks in the learning process. Users are instructed to move between three garages to get informed on the varying aspects of the learning content. First, users are born in the *reception garage* where they are welcomed and introduced to the terminology, problem and objectives with simple tasks. Following this, they are instructed to move into the *chemical garage* to learn about the theory and the case study including interaction 3D visualization of geometry with accompanying tasks. Finally, they come to the *simulation garage* to learn fundamentals on the methodology of CFD with case-specific instructions. Module#1 can provide an engaging meaningful activity that methodically resembles a real-life experience. Because the learning experience covers varying aspects of engineering, it is imperative to let users make distinctions between these aspects using the garage concept. Moreover, we originally designated a *social garage* to highlight engineering competencies and transferable skills such as critical thinking, teamworking, decision-making and time management. We also aimed at providing an environment to interact with users in the virtual space, such as multiplayer in the context of the metaverse. However, in the current state of the prototype, this garage is inactive due to concerns over exposure time.

Module#2 is the assignment with CFD simulations to solve problems introduced at the end of Module#1. We followed a simplistic approach to designing a greyish virtual room – as a simulator – to get users focused on simulation data instead of distracting them with surrounding irrelevant digital content. Unlike Module#1, users can move only in a confined area mostly around simulation data to make logical interpretations. Users work with pre-computed CFD simulation data to interpret findings and make decisions to satisfy stipulated constraints in the learning activity. Having filled the decision-making panel popping up at the end of Module#2, users can compare their answers to the desired ones, and the entire learning experience comes to an end. Optionally, before quitting the Virtual Garage, users can also retrospectively turn back to simulation data to comprehend the reasonings behind the desired answers. A summative assessment weighs the learning outcomes in Module#2. As an extension to the summative assessment, we see the added value of conducting an oral interview either immediately after or at another moment. In this way, lecturers can get more insight into the learning experience by having an internal evaluation of the learning material and activity. In addition, a learning analytics dashboard can be embedded in the learning experience to timely present overall

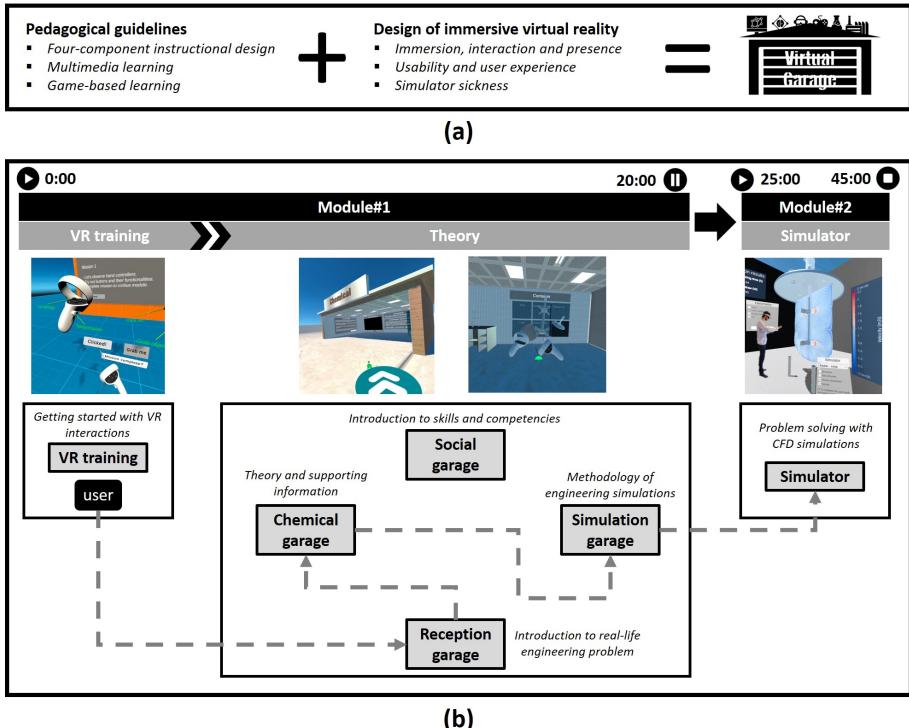


Figure 5.1: The Virtual Garage concept including a list of design guidelines utilized in the conceptualization (a); schematic illustration of modules of the Virtual Garage in detail (b). The user's trajectory is represented with dashed lines.

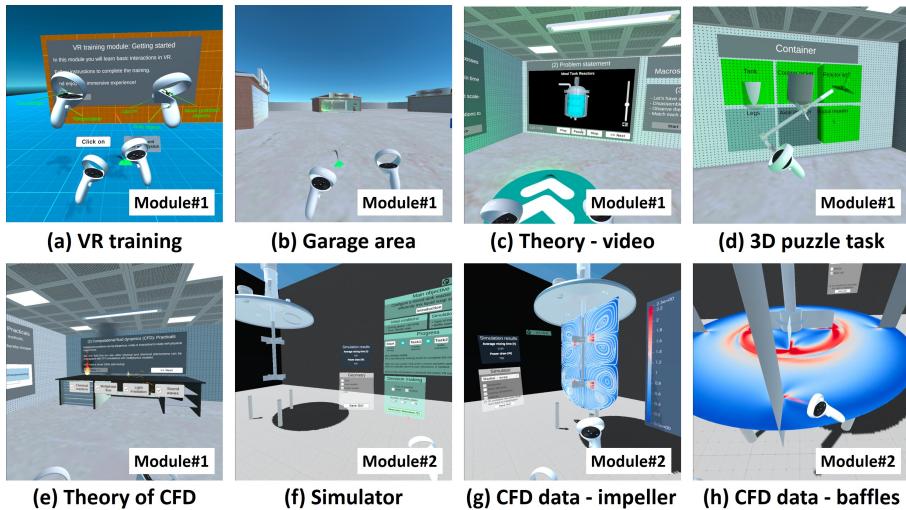


Figure 5.2: Screenshots from the Virtual Garage.

performance. Both modules take approximately 20 min to complete. Users are strongly advised to take a five min break between modules by taking the VR headset off to reduce the potency of simulator sickness.

Fig. 5.2 demonstrates screenshots from different scenes of the Virtual Garage application. It is composed of 15 conceptual case studies, such as micro-learning nuggets, to provide immersive learning experiences on complex engineering topics, relatively focusing on mixing and process intensification in chemical engineering. Two out of 15 case studies are prototyped and ready to test with students. In this study, we perform user studies with the case study Case#6: design a stirred tank reactor. Users are asked to configure a stirred tank reactor to efficiently mix liquid soap solution using design and operating parameters. Several learning objectives are given to deepen their knowledge of the effect of viscosity, type of impellers, rotational speed and baffle plates, which are detailed in the Supplementary information for Chapter 5. The Virtual Garage is developed with Unity Game Engine and deployed on Meta Quest 2 VR headset. In the Supplementary information for Chapter 5, a walkthrough video of Case#6 on YouTube and VR software for Meta Quest 2 on GitHub are freely accessible.

Table 5.1: Participant demographics (n=24).

Characteristics	Items	Number	Percentage (%)
Gender	Male	20	83
	Female	4	17
Age	22-24	6	25
	25-27	7	29
	28-31	11	46
Current education	Master	7	29
	PhD	17	71
Any experience in CFD	yes	8	33
Any experience in VR	yes	17	71
Any experience in CFD with VR	yes	0	0
Like gaming	yes	15	63

5.3 Materials and methods

5.3.1 Participants

Experiments were conducted at the department of chemical engineering at KU Leuven. Participants filled in a pre-test before the experiment to score their interest and experience in VR, CFD and gaming together with demographics including gender, age and educational level. As illustrated in Table 5.1, 24 participants (20 male and 4 female) from the graduate school took part in the testing, of which 17 were Ph.D. students and 7 were Master students. No participants dropped out during the testing. Participants' age varied from 22 to 31 ($M = 26.54$, $SD = 2.77$). Participants had diverse interests and experiences in VR, CFD and gaming from novices to experts. No one had previously used a VR application with CFD simulations.

5.3.2 VR setup

We developed and utilized the Virtual Garage application to evaluate usability and user experience in different modules of the application to understand and improve the overall quality. The Virtual Garage is composed of two subsequent modules, Module#1 and Module#2, as shown in Fig. 5.1. Module#1 is composed of VR training and theory sections. Module#2 is the assignment with CFD simulations to solve problems introduced in the theory. To develop the Virtual Garage, we utilized the Unity game engine with several built-in and external packages. CFD simulations were calculated in a workstation

with OpenFOAM and COMSOL v5.6, thus facilitating a co-simulation pipeline. CFD simulation data was integrated into Unity using an extract-based data processing approach [168]. The VR experience was deployed on Meta Quest 2 VR headsets.

5.3.3 Experimental methods: procedure and conditions

We pursued a mixed methodology to analyze, interpret and critically reflect on measured scales. Several standardized tests were employed together with self-reported questionnaires and a semi-structured interview. A five-point Likert scale was utilized in this study. Before the actual testing, we performed a pilot study with 5 internal staff showing diverse backgrounds somehow related to the Virtual Garage concept. The pilot study improved the application and helped in the design and validation of the experimental materials and methods.

Evaluation methods

Literature previously showed proven methodologies to examine the quality of immersive virtual reality applications based on usability, user experience, task load and simulator sickness [195]. These are crucial quantitative scale to facilitate optimal quality for users before diving into learning and task performance. Most obviously, quantitative analysis has its limitations to interpret underlying factors on overall score. We, therefore, employed a mixed methodology to dig into findings blending quantitative and qualitative instruments.

Pre-test: Participants filled out a pre-test to express their experience in and interest in VR, CFD and gaming along with demographic information. This enabled us to examine the effect of independent variables on various other scales measured in the present study.

Usability: System Usability Scale (SUS) was chosen to evaluate the ease of use of a system as being a massively applied reliable standardized test in the literature [196]. The SUS consists of 10 items to quantitatively analyze the usability of digital products and services by means of learnability, efficiency, memorability, errors and satisfaction. Based on the SUS, we can understand the current state of the VR application in terms of usability, and detect the subscales that can be improved.

Task load: The task load is an imperative metric to deliver digital content in an appropriate way when it comes to educational settings. Despite its original application for aviation, Nasa-Task Load Index (NASA-TLX) has become a well-known multi-dimensional scale to predict task load from cognitive, affective

and behavioral aspects in different domains [197]. By using NASA TLX, we aim at comprehending changes in task loads that design parameters may cause.

User experience: A good user experience is key to producing engaging, interactive products. We applied the User Experience Questionnaire (UEQ) which has high scale reliability and validity, as well as being a broadly utilized scale to measure the pragmatic and hedonic quality of user experience [198]. UEQ has both default and short versions. The default version is composed of 6 scales and 26 items, which requires a certain amount of time for dependent paired tests. The short version only comprises 3 scales and 8 items, and can provide a rapid evaluation to quantify user experience for different variants of the same product such as modules in our study.

Simulator sickness: The immersive VR can induce both physical and cognitive side effects that negatively influence users' well-being. The Simulator Sickness Questionnaire was utilized in this study since it is the most widely utilized scale to examine undesirable side effects arising from immersive VR [193].

Self-reported questionnaires: During the pilot tests we identified some metrics that cannot be directly answered by standardized scales. Therefore, participants were asked to subjectively report their experience with technology and content using self-reported metrics. This way, we can further probe and interpret the outcomes of standardized tests.

Semi-structured interview: In addition to the standardized and self-reported questionnaire, a semi-structured interview was conducted to interpret the outcomes of questionnaires beyond their limited quantified results. The interview consisted of multiple items to explore likeness, interest, redundancy and quality of CFD visuals, potential improvements, implementation in education and personal review.

Data collection

Prior the study, an ethical approval (G-2021-4281-R2(MAR)) was obtained from the ethics committee at KU Leuven to comply with standards for the processing of personal data in academic contexts. It strictly adheres to the requirements of the General Data Protection Regulation (GDPR) and other applicable laws issued by governing bodies. Barring interviews, all data were collected online on a laptop PC provided to participants during the experiments. Interviews were conducted at the end of the experiments through which the researcher took notes from oral feedback given by each participant.

Testing procedure

Experiments were performed in January and February 2022. At that period, the COVID-19 pandemic was still strictly limiting in-person gatherings. Therefore, national and regional safety measures with regard to COVID-19 were applied during the experiments such as proper ventilation of the testing environment, disinfection of equipment and social distancing. Due to safety measures and a limited amount of hardware, participants individually attended the experiments along with the researcher to guide them throughout the entire testing.

Having participants welcomed at the testing place, a short introduction was given about research, ethics, the Virtual Garage application and intended learning objectives. Following this, a consent form was signed by participants, where necessary instructions were provided on their voluntary participation, experimental procedure, data collection, potential risks and discomforts, anonymity and confidentiality. Participation was voluntary, no incentives were given.

Since we did not concentrate on learning in this stage of the research, participants were advised to ask anything content-wise that they struggled with in VR. The experiment started with the pre-test. Then, they were introduced to the VR hardware with relevant personalization settings and started running Module#1 in VR. Right after the completion of Module#1, participants took the VR headset off and answered standardized and self-reported questionnaires on laptops while having a short break. Later, they turned back in the VR and completed Module#2. The same questionnaires were answered after the completion of Module#2 together with additional self-reported questionnaires on CFD content, overall experience and user behavior toward technology. A semi-structured oral interview was performed at the end of the experimental session. The entire procedure approximately took two hours per participant.

5.3.4 Data analysis

Data analysis was carried out separately for quantitative and qualitative data. In the end, quantitative data was mixed with qualitative ones to further explore and interpret analytic findings. Quantitative data, including standardized tests, were analyzed using the relevant guidelines provided by developers. Statistical analysis was performed so as to determine statistical significance by applying descriptive and inferential statistics, as well as (non)parametric analysis. All the analyses were performed using the R programming language for statistical computing. On one hand, mean (M), median (MD), and standard deviation (SD) were calculated to summarize the characteristics of datasets as a part of

descriptive analysis. On the other hand, inferential statistics were utilized to test several hypotheses arising from the research questions. Shapiro-Wilk test was run on all data to confirm the central limit theorem and normal distribution. To compare Module#1 and Module#2, we used the same sample from the population. Thus, it was advised to apply a dependent test for paired samples. If the data is normally distributed, we used paired t-test, and otherwise Wilcoxon Signed-rank test. Likewise, to analyze correlations among modules, experience and demographics, it was recommended to use Pearson correlation for normally distributed data whereas Spearman correlation for non-parametric analysis. The results presented in this study were considered statistically significant when probability $p < 0.05$, marked as bold and asterisk (*).

Qualitative data were analyzed given the concept of thematic analysis [199]. A codebook was developed to structure interview data, through which themes and subthemes were purposefully created. We also quantitatively summarized the qualitative data to point out frequencies of coded themes and subthemes.

5.4 Results and discussion

This section concurrently presents and discusses qualitative and quantitative results to facilitate a coherent understanding of our findings.

5.4.1 Usability analysis

Fig. 5.3 shows the mean SUS scores for each module. Both Module#1 and Module#2 were well received by users resulting in mean scores of 74.37 ($MD=75$, $SD=10.01$) and 73.85 ($MD=76.25$, $SD=10.16$), respectively. A SUS score above 68 is considered acceptable [196] and good [200].

To examine the differences between modules, a statistical analysis was performed. The Shapiro-Wilk test revealed that Module#1 is normally distributed ($p = 0.252$), whereas Module#2 is not ($p = 0.037$). Thus, the non-parametric Wilcoxon signed rank test was chosen. According to the Wilcoxon signed rank test no statistical significance was observed between modules ($p = 0.684$).

Moreover, in order to examine the effect of experience and interest on usability, we performed an additional analysis to detect potential correlations. Since the dataset is not normally distributed, we used the Spearman correlation. Only two correlations were statistically significant which were directly related to the SUS score of Module#2. It was revealed that the ones, who find CFD simulation data intuitive on desktop settings, rated higher usability in Module#2 ($p =$

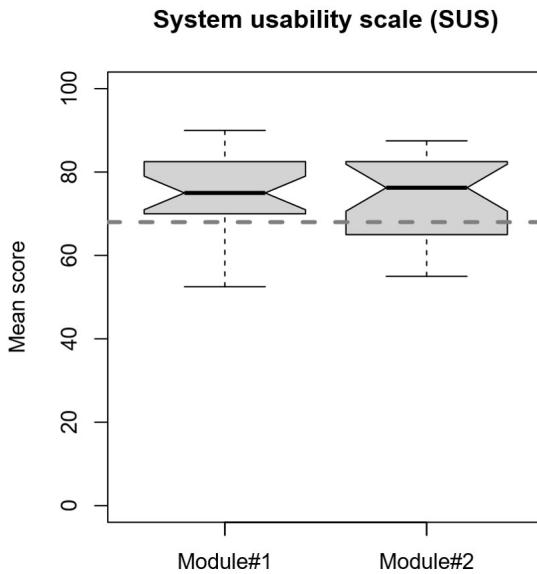


Figure 5.3: The SUS scores with descriptive statistics. The dashed line thresholds acceptable SUS score above 68.

0.037*, $r = 0.426$). Likewise, it was observed that the ones, who find a desktop setting to visualize 3D data difficult, also reported lower usability in Module#2 (**p = 0.014***, $r = -0.493$). All in all, these two correlations showed that prior experience with simulation data and 3D models on desktop settings positively reflected on users' abilities to operate Module#2.

The SUS score is composed of 10 items as shown in Table 5.2. Despite the differences among items of modules, neither of them is statistically significant. Interestingly, *need support* and *inconsistency* items were increased by 7.8% and 10.5% in Module#2, respectively. Although these variations are not statistically significant, we further considered blending interview data to possibly clarify what might be the reason behind these increases. The qualitative analysis outlined imperative findings to explain these differences through 3 themes; CFD scene features, interaction with GUI, and instructional design.

In terms of need support, some participants - specifically mentioned for Module#2 - needed supportive information to interpret and compare simulation data. They proposed help buttons to remind them the important terminologies; for example, "what is the Eddy diffusivity?". Besides, they also demanded a comparison option to put two different data side by side in the same scene,

Table 5.2: The SUS items in modules with relative differences.

Item	Module#1	Module#2	Diff (%)
Use frequently	3.67	3.67	0.00
Complex	2.00	1.96	-2.08
Easy	4.08	4.04	-1.02
Need support	2.13	2.29	7.84
Well integrated	4.17	4.17	0.00
Inconsistency	1.58	1.75	10.53
Learn quickly	3.92	4.04	3.19
Cumbersome	2.17	2.25	3.85
Confident to use	3.67	3.75	2.27
Need to learn a lot	1.88	1.88	0.00

thereby simultaneously comparing differences for two design parameters. Some also mentioned the need for more signaling and procedural information to guide them through multimodal CFD data in Module#2. Conclusively, users needed more support in Module#2, therefore, the relevant item in SUS was increased.

The inconsistency item was increased in Module#2. Similar to the prior item, some participants mentioned specific features in Module#2 that caused an increase in inconsistency. Notably, users had trouble interacting with the GUI in Module#2, as well as the operations of buttons. In order to switch between different simulation settings, we used the word "initialization" in the dropdown menu, which was not clear for some users despite relevant instructions being provided in the digital environment. It was also revealed that some users were uneasy with the dropdown menu itself, thus finding it unintuitive. Furthermore, the GUI in Module#2 is grabbable, which means that users can grab and relocate GUI in the virtual environment to personalize their experience. There was a button attached to the GUI to manually "save" the latest location. Nevertheless, users forgot to click on the save button, or simply did not understand its function, even though necessary instructions were provided on the same GUI. All in all, some components of the GUI were found unintuitive in Module#2, and this was negatively reflected in the inconsistency item of SUS. We believe that using a tablet-like GUI attached to the hand controller can tackle problems with interactions. A similar solution was previously recommended by a user study with regard to the qualitative feedback [37].

Thanks to the mixed methodology, it is obvious that the SUS score can be increased by providing more help, supportive and procedural information on the simulation data, as well as making GUI more intuitive and accessible. Not only need support and inconsistency, but also other items of SUS can be

positively affected by these improvements if the same is applied to the entire VR experience.

To sum up, our initial guess on the increases of *need support* and *inconsistency* was simply related to the multimodal simulation data, such as 3D volumetric data, 2D visuals, graphs, charts and numerics. In contrast to this, our findings showed that usability was the main reason behind the negative trends in the SUS score of Module#2. It is also worth mentioning that all participants rated the CFD data in Module#2 as intuitive and interactive.

5.4.2 Perceived task load

NASA Task Load Index (NASA-TLX) is applied to quantify the perceived task load of digital systems operated by humans. It measures mental demand, physical demand, temporal demand, performance demand, effort and frustration. We compared the task loads of modules in the Virtual Garage, particularly focusing on how the task load would be impacted in Module#2 due to the use of simulation content and relevant given tasks such as data exploration and decision-making. In this study, unweighted NASA-TLX was used as a sensitive measurement of task load as the weighted version [197]. The NASA-TLX scores overall task load in six consecutive categories; low (0-9), medium (10-29), somewhat high (30-49), high (50-79) and very high (80-100) [201].

Fig. 5.4 shows overall scores measured with the NASA-TLX test to assess the task load in the modules. Module#1 overall scored medium task load (27.8%) whereas Module#2 scored somewhat high task load (36.8%). Results showed that participants overall found Module#2 more demanding than Module#1, with a 33.4% increase in the average score. Only physical demand was lower in Module#2. This trend can be explained by the simplistic design of the simulation environment in Module#2, in which users are centered around simulation data in a confined virtual space. Users were not supposed to move farther distances in the virtual space since the mere focus was to closely explore simulation data to make decisions. In contrast, in Module#1, users move inside the virtual space among garages to receive supportive information and complete tasks to reach Module#2.

Statistical significance was analyzed to more in depth examine the comparison between modules. It was observed that the average score was normally distributed ($p > 0.05$) while all of the subscales were not normally distributed ($p < 0.05$). According to the paired sample t-test, the differences between the average score were found to be statically significant ($t = -4.786$, $df = 23$, $p < 0.001^*$). The task load significantly increased in Module#2, which lends support to our initial guess. Furthermore, the Wilcoxon signed rank test was

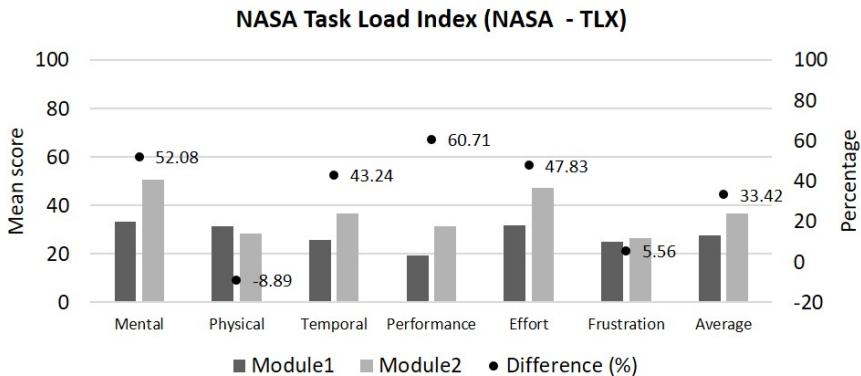


Figure 5.4: The NASA-TLX test measuring task load in the modules.

applied to examine statistical significance in subscales. It was revealed that the mental demand ($p < 0.001^*$), temporal demand ($p = 0.025^*$), performance demand ($p = 0.023^*$) and effort ($p = 0.004^*$) were significantly increased in Module#2, whereas the physical demand ($p = 0.388$) and frustration ($p = 0.941$) were not significantly changed. This clearly substantiates that even though users were more challenged in Module#2, they did not get frustrated at all.

To further interpret the quantitative analysis of the task load, we utilized the interview reports. Mental demand significantly increased (52%) in Module#2. Users reported the need for supportive and procedural information. They required guidance to properly interpret the simulation data, and subsequently make logical decisions to solve the problem introduced in Module#2. The tasks in Module#1 were generally simple puzzle games upon the abstract content such as word matching for problem description and geometry dissemble, in which mental demand was far less than in Module#2. Also, a group of participants indicated that they sought to assist features to visualize simulation data such as setting the view direction for different coordinates and angles on click, as well as a comparison mode to put two data side-by-side. It was also requested to make a virtual notebook available for users in Module#2, where they can take notes and return back to them when it comes to decision-making. Otherwise, users either forgot or several times turned back to the same data to memorize their decision. In addition, some users were uneasy with the GUI and its operations due to its unintuitive and inconsistent features. A discussion on this was made in the previous section. We believe that all these qualitative reports point to the probability of an increase in mental demand in Module#2. On the whole, users

needed more instructional support to understand and interpret simulation data along with features to reduce cognitive loads such as a comparison view and virtual notebook in the support of a well-structured decision-making process. Our results are consistent with previous findings in the literature concerning non-experts' interaction with CFD data [37].

Similar to mental demand, effort and performance demand were significantly increased in Module#2. We believe that the abovementioned reasons behind the increase in mental demand also played a direct role in increasing effort and performance demand in Module#2. In addition, the temporal demand also increased in Module#2. It is noteworthy that in Module#2 users had a timer counting down from 20 min, which was not available in Module#1. Interestingly, interview reports unveiled that some participants got stressed due to the timer. This might be one of the reasons behind the increasing temporal demand together with mental, effort and performance subscales.

Furthermore, in order to statistically examine the relation among subscales, we performed a test to correlate subscales to each other. Table 5.3 summarizes statistically significant correlations for modules and relevant subscales with the Spearman correlation for non-parametric analysis. Mental – Effort and Effort – Frustration are positively correlated in both modules, which provides further evidence on our above interpretations of qualitative data on the increase of mental demand and effort. In Module#1, Performance – Effort is also found to be positively correlated, yet this is not the case in Module#2. In addition, Mental – Temporal, Mental – Frustration and Physical – Frustration are positively correlated in Module#2, but not in Module#1. The results from such analyses should be interpreted with caution. For instance, although the frustration was not significantly changed between the modules, it was linked to the mental demand in Module#2.

As performed in the usability analysis, we statistically investigated the effect of experience and interest on the perceived task load. Since the dataset is not normally distributed, we used the Spearman correlation. No significant correlation was identified for the average task load score in both modules. Nonetheless, there were significant correlations detected for subscales. The degree of frustration in Module#2 is negatively correlated with the ones experienced in 3D modeling on 2D desktop settings ($p = 0.022$, $r = -0.466$). The more users are experienced in 3D modeling, the less frustrating Module#2 becomes for them.

Lastly and unexpectedly, there was a significant positive correlation between mental demand in Module#2 and expertise in CFD ($p = 0.034$, $r = 0.433$). In other words, the ones who are experienced in CFD reported higher mental demand in Module#2. The interview report might shed light on this unexpected

Table 5.3: Testing correlations on subscales of the NASA-TLX.

Correlated items	Module#1		Module#2	
	p	r	p	r
Mental - Effort	0.010*	0.516	0.001*	0.743
Mental - Temporal	-	-	0.039*	0.424
Mental - Frustration	-	-	0.012*	0.502
Physical - Frustration	-	-	0.007*	0.537
Performance - Effort	0.024*	0.460	-	-
Effort - Frustration	0.011*	0.511	0.003*	0.572

finding. CFD data available in Module#2 were well sufficient to make a final decision to solve the problem. However, the ones experienced in CFD simulations orally reported that they needed more data and data processing options to come to a conclusion such as 3D iso-surfaces, transient results, slices and cutlines from different coordinates, various scaling options and side-by-side comparison. In general, someone experienced in CFD simulations iteratively carries out data processing work to find optimal post-processing out of the entire CFD dataset. These post-processing are then utilized in the decision-making process. Having in advance final post-processing without any interactive option for reprocessing and data exploration, CFD-experienced users might be challenged due to limited features of the system which is inherently against the workflow they are used to apply, thus scoring higher mental demand in the task load. More on the cognitive part of task load could be further factored in a scale specifically developed for immersive VR, thus providing a better understanding of hindering effects [202].

5.4.3 Quality of user experience

Fig. 5.5 shows the UEQ scores of modules together with a benchmark scale to assess the qualities of the user experience. Both modules scored good overall, even though pragmatic and hedonic quality resonated between above average and good. Pragmatic quality covers the items of supportive, easy, efficient and clear, while hedonic quality is composed of exciting, interesting, inventive and leading items.

The summary of the UEQ scores can be found in Table 5.4. While Module#1 scored higher in pragmatic quality, Module#2 took the lead in hedonic quality. Statistical analysis with the Wilcoxon signed rank test showed that only the change in pragmatic quality is substantial.

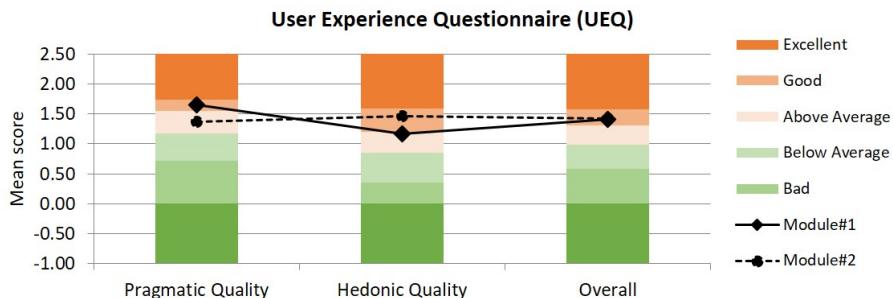


Figure 5.5: The UEQ comparing the user experience in modules against the benchmark scores.

Table 5.4: Summary of the UEQ scores.

Item	Pragmatic Quality	Hedonic Quality	Overall
Module#1	1.66	1.17	1.41
Module#2	1.38	1.47	1.42
Difference (%)	-20.45	20.21	0.55
Statistical significance	p = 0.048*	p = 0.109	p = 0.930

To increase our comprehension of changes in scales, we also took a closer look at items in each scale as summarized in Table 5.5. No statistical significance was obtained for the items in pragmatic quality, despite the significant change in modules. However, it was observed that items *supportive* and *clear* arguably dropped in Module#2, 42.1% and 52.9%, respectively. Reductions in both may be accordingly reflected in the pragmatic quality in Module#2. As presented and discussed in the previous subsections, some interviewees indicated the need for supportive and procedural information to guide them in Module#2, particularly in the interpretation of simulation data and assistance for decision-making. Similar to this, users also described Module#2 as less clear than Module#1. This may be due to unfamiliar terminology utilized in the GUI and its unintuitive functionalities.

As previously presented, the SUS has similar items *need support* and *inconsistency*, which increased in Module#2 by means of usability. This pattern can provide considerable insight into *support* and *clear* items, for which users sought more in Module#2. All in all, the pragmatic quality was significantly

reduced in Module#2, which means that users found it less supportive and clear. It is worthwhile noting that, unlike initially thought, the reduction in pragmatic quality is not because of the simulation data but because of issues in usability and user experience.

Concerning the hedonic quality, also detailed in Table 5.5, the exciting item showed a statistically significant increase in Module#2, whereas no significant difference was observed for other items. The exciting item increased by 44.4% in Module#2, alongside the interesting item which increased by 30.4%. Yet, due care must be exercised in the discussion because no statistical significance was detected in the overall hedonic quality scale. Several participants expressed their positive feelings on immersive interaction with 3D reactor geometry and volumetric CFD simulation data in Module#2. Some participants even extended their comment to Module#1, for which they hardly ever found the immersive features of VR well exploited as initially expected. However, they were eventually satisfied with Module#2 due to the direct immersive and interactive experience with reactor geometry and simulation data. We presume that these findings can underline just how exciting Module#2 was compared to Module#1, which is basically a structured environment mostly including multimedia to deliver required supportive information with the playful tasks before proceeding with the CFD simulation in Module#2. In addition, all users directly reported that they found the simulation data intuitive and interesting. This positive feeling was clearly indicated in the interesting item.

All in all, it would appear that increasing pragmatic quality for Module#2 and hedonic quality for Module#1 can most likely result in better user experiences.

Moreover, our results share a number of similarities with a recently published framework that identifies a telepresence continuum between atomistic and holistic VR experiences [14]. The former, in which pragmatic quality is higher, requires less telepresence and is fundamentally aimed at completing a procedural task successfully. This resembles Module#1 in the Virtual Garage. The latter, in which hedonic quality is higher, resembles more a real-life experience giving a high degree of telepresence. Module#2 is not dissimilar to the definition of holistic experience. Our results showed that users rated higher hedonic quality and lesser pragmatic quality in Module#2 than in Module#1. These findings correlate favorably with the framework [14] and further support the variation in the user experience based on telepresence.

Furthermore, another test was performed to correlate the user experience to demographic data. Spearman correlation was chosen for the non-normal distributed datasets. The pragmatic quality in Module#2 showed a significantly negative correlation with the ones who ranked that using a desktop setting to visualize 3D data is difficult ($p = 0.013^*$, $r = -0.5$). In other words, participants

Table 5.5: Summary of the UEQ item scores.

Items		Module#1	Module#2	Difference (%)
Pragmatic quality	Supportive	1.69	1.19	-42.11 (p>0.05)
	Easy	1.63	1.56	-4.00 (p>0.05)
	Efficient	1.69	1.69	0.00 (p>0.05)
	Clear	1.63	1.06	-52.94 (p>0.05)
Hedonic quality	Exciting	0.94	1.69	44.44 (p = 0.0197*)
	Interesting	1.00	1.44	30.43 (p>0.05)
	Inventive	1.75	1.75	0.00 (p>0.05)
	Leading edge	1.00	1.00	0.00 (p>0.05)

who find desktop settings to visualize 3D data difficult are also challenged in Module#2. Again, experience in 3D modeling might be the important factor here since these participants are more familiar with 3D models and simulation content, and also might have developed higher cognitive skills to work with them.

5.4.4 Simulator sickness and well-being

The simulator sickness questionnaire (SSQ) calculates total simulation sickness with three different subscales; nausea, oculomotor disturbance and disorientation. A total of 11 participants out of 24 reported sicknesses. 7 out of 11 participants, who reported sicknesses, did not use any VR experiences prior to this study, and the rest had only one-time experience. Table 5.6 lists SSQ scores for different subscales and total simulator sickness. All participants successfully completed the entire VR experience without having major discomfort.

Ten participants mentioned sicknesses in Module#1, and subsequently seven of them continued reporting similar side effects in Module#2. One participant, who did not mention any sicknesses in Module#1, reported sicknesses in Module#2. Overall, the degree of sickness significantly lowered in Module#2 compared to

Table 5.6: The SSQ mean scores with subscales.

SSQ	Nausea	Oculomotor disturbance	Disorientation	Total simulator sickness
Module#1	17.49	18.95	27.26	23.53
Module#2	8.35	10.42	11.60	11.53

Module#1. Even though debates on qualitative analysis of simulator sickness are not yet well settled, recently published research showed that virtual reality environments with an SSQ score below 40 are assumed to be safe in terms of simulator sickness [193]. This assumption makes both modules qualified in terms of health aspects.

Why did the sickness scores decrease in Module#2? Design guidelines may have a vivid answer for this trend. In Module#1, users move in VR via teleportation among different virtual buildings, such garages, throughout the experience. This approach was abandoned in Module#2 since we want users to focus toward simulation data, thereby less movement to experience in the virtual space. Module#2 also has a simplistic design in which users are centered on simulation data in a confined space without any distractive surrounding digital assets. These may be the reasons behind the reduced level of sickness. In addition, the scores might be lowered due to the experience they gained in Module#1. No statistical analysis was performed due to discontinuous and segregated datasets.

In the interview session, three participants verbally conveyed perceived physical disturbances caused by the headset, thus affecting their well-being during the VR experience. These three participants also reported sicknesses via SSQ. All of them were novices to VR applications. Simulator sickness can also be triggered by not properly worn VR headsets. Hence, it is imperative to give a short demonstration to participants about how to wear and accordingly adjust the VR headset, and to let them a moment to explore the hardware while finding the optimal setting for their physical comfort. Module#1 comprises a VR training section, in which users do engage with hand controllers and interactions in the virtual space. Though not being applied in the Virtual Garage, the training section can also be utilized to demonstrate what kind of adjustments users can actually do to properly wear VR headsets, and to find the appropriate settings. This may further help reduce to the potency of simulator sickness caused by physical disturbance.

5.4.5 Qualitative feedback

Most of the qualitative data were already blended with quantitative data in previous sections to explore and interpret the reasonings behind user behavior. However, there are still some valuable comments given by participants left that can help us further probe the interesting features of the Virtual Garage. These are discussed in this section.

Thematic analysis: remaining remarks

Seven different themes and 37 subthemes were purposefully generated using a thematic analysis method with a codebook as illustrated by the number of subthemes and frequencies in Fig. 5.6. Checking on the frequencies of themes in the codebook, some 60% of user feedback is made of *CFD scene features*, *interaction with headset and hand controllers* and *interactions with GUI* themes. This highlights the imperativeness of the qualitative analysis to pinpoint important design parameters. Because immersive virtual reality learning environments are made of truly diverse and subjective elements, standardized questionnaires may not always cover underlying factors.

Interesting remarks can be made on the features of Module#1. The VR training at the beginning of Module#1 was perceived as helpful by the participants. No instructions about operations were given to the participants before the VR experience. Participants learned hand controllers and interactions using the VR training module as a part of a holistic VR experience. This helped to save time and also get participants playfully engaged with VR before dealing with the educational content.

Besides, some participants liked watching content videos in VR and find them engaging despite their negative initial perceptions. Participants also liked and found engaging and intuitive the 3D geometry disassembly puzzle game, as a playful task completed in Module#1 to understand the components of the reactor. Surprisingly, multiphysics animations in the simulation garage were described as being redundant by participants since they were not directly related to the learning content. Our intention to add these animations was to show the capabilities of multiphysics CFD simulation through visual but abstract 3D animations such as smoke propagation and sound waves.

Interviewees also commented on the entire Virtual Garage experience. They found it credible, holistic, fluid and immersive. These comments are in line with the perceived impressions that we want to trigger within the Virtual Garage. Another remarkable comment was on timing and its procedure, which was

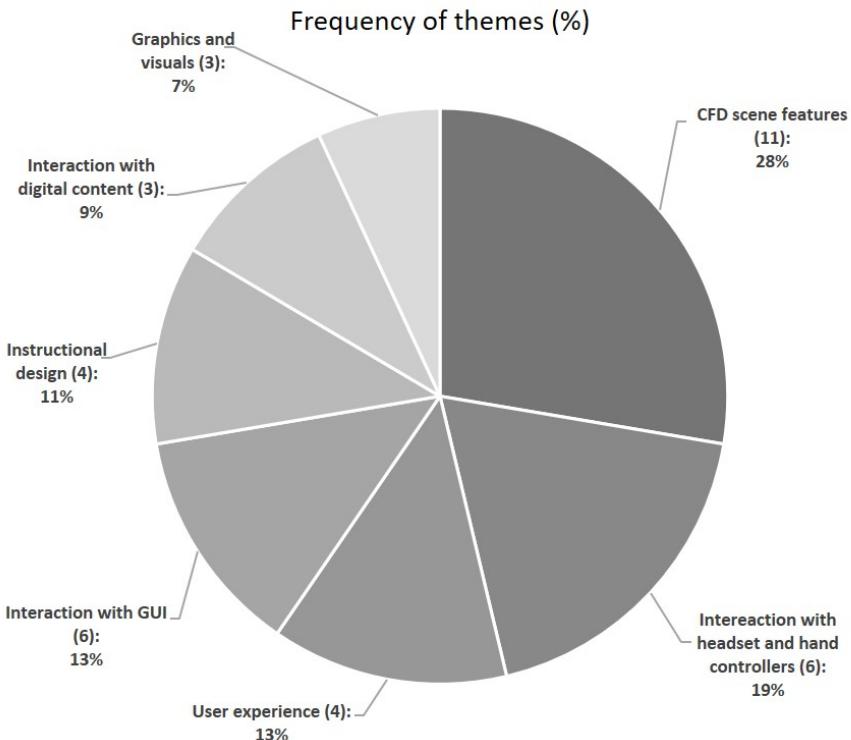


Figure 5.6: Thematic analysis with number of subthemes and frequencies (%).

rated as optimal. Users were given 20 min per module with a five min break in between to diminish simulator sickness.

Furthermore, hand controllers in the Virtual Garage are utilized to interact with GUI and digital content, for example grabbing reactor components. The rest of the operations were conveyed through GUIs available in modules. Participants found this approach relatively easier than other VR experiences they were previously exposed to. Therefore, they rated interactions in the Virtual Garage simple and easy to control. Although, some users forgot to use the thumbstick, which had the functionality to move a grabbed object in the virtual space, even if it was also a part of the VR training at the very beginning. This implies that at least some hand controller-related procedural information could be conveyed in the modules to remind users of the functionalities of buttons.

Another intriguing finding was about audio instructions in the Virtual Garage.

Inherently, we design all audio instructions compulsory to listen to even if a written script was made available in the same scene. Some users found this setting redundant and expressed their intention to skip audio instructions - or at least make them optional to listen - if it is the same as the written script. In addition, some users wanted to change the audio volume and found the default volume set to either quiet or loud. Meta Quest 2 has a button at the bottom of the headset to adjust the audio volume. Neither before the VR experiment nor in the VR training in Module#1 this feature was highlighted to participants. Therefore, our advice here is to give instructions about this button or alternatively provide a headphone which can also help them be isolated from external sounds. Lastly, no negative feedback was collected on background music, for which we were initially concerned that some users might get interrupted.

One participant asked for an option to operate the VR experience while seating. In this study, all participants run the test while standing to mitigate any difference that may arise from this setting. In practice, seating should work since users move in the virtual space via teleportation. A recent study compared both conditions and found no statistical differences between standing up and sitting [188]. In the future edition, users may be accordingly instructed to choose the preferred physical setting. The most obvious advantage of the seating position is that less physical space is required for the VR testing because users would be safe and static in a confined area. Likewise, some participants demanded more precise moving in the virtual space. In this version of the Virtual Garage, users are let freely teleport. However, some stationary points could be spread through the virtual place where users are supposed to be engaging with the virtual content. Instead of moving freely, users click on the stationary point and are directly teleported to the relevant location.

Interesting comments were also revealed on the quality of graphics and colors. Some users expected a higher quality digital content. Even though Meta Quest 2 is a decent VR headset in terms of computing power, it would be quite challenging to increase quality for the sake of realism. It is more important to optimize graphics to enable a fluid VR experience without having any latency and drop in the frame rate. Eventually, it is a trade-off to be optimized between graphics quality and frame rate.

Finally, some users reported on colors, for which they preferred more distinctive colors – or textures - for 3D models and highlighted virtual content. In the Virtual Garage we carefully chose accessible colors and colormaps for easy interpretation, and people with color and sight disabilities. The same applied to the visual representation of CFD data choosing accessible colormap following a recently published critique on scientific data visualization [194].

Relation of experience and interest

VR novice participants found the VR training helpful to learn controllers and interactions in the Virtual Garage. The headset-related physical disturbance was only reported by novices. They also needed more instructions and signaling to navigate themselves through the virtual space.

The ones, who like playing games, described the VR experiences as holistic and fluid. They expected more specific instructions about tasks to be completed, for example, the puzzle game. They demanded more interactive features such as scaling, side-by-side view, and different view options to analyze CFD data. They also preferred the audio instructions to be optional if the written version is made available in the same scene. They liked the personalization of the virtual environment by moving the GUI.

CFD-experienced participants reported that the immersion and interaction are spatial and 3D, and can help develop cognitive abilities to understand and interpret 3D data. They found the playful animations (fire, smoke, etc.) in the simulation garage redundant and cumbersome. Due to their hands-on experience, they also wanted to be exposed to more data such as 3D data, iso-surfaces, transient data, and representative animations such as how the impeller turns – making it more operable, interactive and playful.

Integration in education: users' perspective

Participants were also asked to give some insights on the implementation of such tools in current educational practices. In general, they agreed on complementary and/or supplementary integration of similar tools to an exercise session for such courses including transport phenomena, microfluidics and broadly engineering design and analysis. Some participants also foresaw its help in teaching CFD and fundamentals of fluid mechanics such as continuum hypothesis, integral relations for a control volume and dimensionless numbers. One participant detailed a scenario to integrate VR in the current educational settings. The participant proposed integrating it into a group activity preferably during an exercise session. Having an imaginary classroom with 40 students, the participant divided students into groups, forming eight groups of five students. Each group has one VR headsets and swaps among each other. In addition, another participant reported that it could be useful for the sake of edutainment to attract young students.

One participant mentioned the potency of the remote utility of the application at home as delivered below:

- "It would be useful to download and use it at home. Instead of going to the real plant you use the VR to get there and learn about engineering."

Using VR only to visualize CFD data was also found an effective interaction to make CFD data intuitive, even if there is no accompanying content in VR. Below are the responses from students highlighting added-value of VR to visualize CFD simulations:

- "Very cool for example chemical design problems, do a simulation with COMSOL, transfer to VR and see the results. This might be helpful there."
- "CFD in VR data helps you understand fluid flow even if you know nothing about the content and simulator."

Overall, participants anticipated the added-value of the Virtual Garage and VR technology in their current educational practices. They remained positive toward the implementation; however, they also conveyed doubtful and contradictory comments on their peers' acceptance of this technology in education.

5.4.6 Self-reported questionnaire

We further added two self-reported items that may not be directly evaluated in qualitative and quantitative analyses according to the pilot study carried out before the experiments. We asked participants to compare modules by means of the help of VR training at the beginning of Module#1 and satisfaction with visual content, as can be seen in Fig. 5.7.

A five-point Likert scale was utilized as in the other questionnaires. VR training was found helpful in both modules and did not show a significant change between them. In contrast, the likelihood of satisfactory visual content was significantly increased in Module#2 ($p = 0.0197^*$). This substantiates our findings via standardized tests that users rated Module#2 more exciting and interesting, the reason behind the increase in hedonic motivation in UEQ.

5.5 Limitations and perspectives

5.5.1 Study limitations

Our study obviously has some limitations. Given that the focus of this study was on the evaluation of usability, user experience, task load and simulator

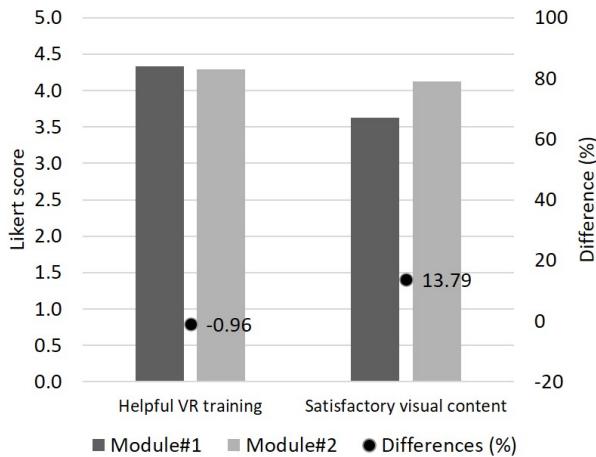


Figure 5.7: Self-reported items.

sickness, we could not provide any remarks on the task performance and learning effect. This may discourage some readers who seek evidence to justify the utility of VR in engineering education. However, it should be noted that this study is the first step toward assessing a holistic immersive virtual reality learning environment with CFD simulations. Hence, we purposefully concentrated on human factors instead of directly moving into task performance and learning assessment.

Due to the holistic but diverse structure of the Virtual Garage, we could not come up with any existing educational practices for comparison. Instead, we compared two modules with and without CFD simulation data to understand its effects on the usability and other measured scales in this study. Alternatively, we could have compared different design features of CFD data in Module#2 such as coloring, scaling option, varying visual representations and instructional design. Several of these features were properly implemented in the Virtual Garage using available literature and guidelines. Nevertheless, our study brought miscellaneous other features under the spotlight that can help learners to interact with simulation data in VR, for example, side-by-side view selection and a virtual notebook. Furthermore, the assessment part in the Virtual Garage (learning analytics dashboard, retrospective feedback, and post-dialogue) was not yet implemented. Hence, we did not provide any results and discussion on performance and learning assessment. We plan to process a set of those in the next version.

Based on a very small-scale pilot study prior to the testing, we found that a qualitative methodology can help interpret quantitative data. Thus, a concurrent mixed methodology was followed in this study, collecting quantitative and qualitative data. Data collection was made at the same time due to our concerns over reaching out to the same portion of population in later time. This left some ambiguities and unjustified findings because a larger population brought a diverse dataset to tackle than the pilot study. If the participants are reachable without paying too much effort after the study, it would suit best to subsequently carry out the qualitative data collection based on quantitative results.

We were able to recruit 24 participants for this set of the study. Due to COVID-19-related restrictions, we had to run experiments one by one. Another challenge was the number of available hardware and sufficient physical space to run experiments. All this obviously limited us to work on a small sample size. Despite this, the study showed interesting results to satisfy posed research questions with reliable data analyses. Participants came from diverse backgrounds in terms of experience and educational level. This also helped us properly evaluate the learning environment and find features to be further improved.

5.5.2 Our perspective

Future work is to firstly consolidate the outcomes of this study and process relevant improvements in the digital environment. On a broader level, in this study, we did not directly measure affective and behavioral factors. However, it appeared that there is a need for investigation of students' technology use and acceptance of newly adapted digital educational tools. As a part of the future work, we are planning to set up another set of experiments to measure task performance, learning and technology acceptance.

There are also a set of twists that remained unanswered and worth investigating. Our findings suggest the following directions for future research. Firstly, researchers may focus on different attributes of CFD data in VR to help nonexperts effectively interpret simulation data. Secondly, more structured and user-friendly authoring tools may encourage practitioners to try and adapt to such digital environments. Thirdly, measuring lecturers' intention to use VR in engineering education seems to be vital to unleashing hindering factors. Besides, comparing in-class and remote use of VR and its effect on learning would be a valuable contribution since remote learning has been increasingly becoming a popular realm. Finally, collaborative features may further be an enabler for remote and social learning given the increasing popularity of metaverse-like educational environments. Not only education but also engineering can also

benefit from multiplayer option to effectively and collaboratively communicate CFD simulation data in immersive VR. See the respective entry for a detailed description of the educational use of metaverse [203].

5.6 Conclusion

The focal point of our work is to investigate the learning effectiveness together with cognitive, affective and behavioral aspects of immersive learning with CFD simulations. To perform a reliable evaluation of these metrics, we initially focus on the assessment of the design parameters in the Virtual Garage concept. Hence, the purpose of this paper is to assess human factors as a first step toward the evaluation of immersive virtual reality learning environments with CFD simulations. Our preliminary analysis has shown promising results regarding the design, development and evaluation of CFD simulations in immersive learning. Considerable progress has been made with regard to the quality of the immersive learning experience with CFD simulations assessing usability, user experience, task load and simulator sickness. Concerning the scarcity of relevant literature to date, our findings and remarks might help developers to find proper guidance in their development journeys.

Future work will focus on improvements in the prototype in the first place. This will ultimately be pursued by a follow-up user study to measure knowledge gain, task performance and technology acceptance. Notably, we aim at measuring technology acceptance due to its comprehensive but structured methodology to figure out what lies behind students' intention to use similar applications by utilizing miscellaneous factors evidenced by literature such as habit, motivation, personal innovativeness, content value and so forth.

Chapter 6

Behavioral intention, perception and user performance in an immersive virtual reality environment with CFD simulations

The chapter is under review in a peer-reviewed journal: *Solmaz, S., Gerling, K., Kester, L., and Van Gerven, T. Behavioral intention, perception and user assessment in an immersive virtual reality environment with CFD simulations.*

Author contributions: S. Solmaz conceived the research, performed the data analysis, interpreted the results and wrote the article. T. Van Gerven, L. Kester and K. Gerling contributed with their guidance and expertise in this work.

Abstract This study explores technology acceptance, perception and user performance of an immersive virtual reality environment with computational fluid dynamics simulations in engineering education. 57 participants from three different institutions tested the virtual reality application. Partial least squares structural equation modeling and inferential statistics were performed to predict and assess interrelations among performance expectancy, effort expectancy, intrinsic value, learning value, self-efficacy, content value, personal innovativeness, flow theory and behavioral intention. Results show that the learning value, content value, intrinsic motivation and personal innovativeness

are underlying factors behind students' intention to use virtual reality. Pairwise analysis indicates that users' perceptions matter and positively affect their attitudes. In addition, the virtual reality application helps students perform significantly better in the post-knowledge test. Findings also highlight that prior experience and interest can affect students' attitudes and behavioral intentions to accept the virtual reality application in education. Our study can guide lecturers and developers to achieve on-target immersive virtual reality learning environments in higher education.

6.1 Introduction

Since the turn of the century, technology has progressively transformed education, and it will undoubtedly become the main driver of educational practices in 10 to 15 years [5]. Notably, augmented reality (AR) and virtual reality (VR) technologies have recently been receiving much attention due to the advanced levels of immersion and interaction on cognitive, affective and behavioral levels [6, 13, 14]. VR headsets are affordable technologies for both institutions and individuals today thanks to the recent advancements in hardware and software. Nevertheless, the adoption of VR headsets particularly in engineering education is facing a stiff challenge due to a lack of relevant digital content and, more broadly, of reliable guidelines in the design, development and implementation of such content [13, 18, 19, 20, 15, 204, 21].

Computational fluid dynamics simulations (CFD) are physics-based numerical solvers widely utilized in engineering design and analysis. They help accurately predict fluid flow with relevant physical and chemical phenomena. Both low and high-order cognitive skills with analytical approaches are required to solve engineering problems with CFD simulations. Performing a complete CFD simulation project requires skills in engineering, computer science and mathematics, thus being a multidisciplinary tool in need of a certain level of expertise. CFD simulations have been increasingly utilized in VR applications to reduce the entry barrier for non-experts [178, 16, 205]. Several proofs-of-concept have been demonstrated in immersive technologies with high-fidelity engineering solutions from medical experts [36] to farmers [37]. Apart from technical aspects of integrity, human factors have been recently taken into account to provide better user experiences with CFD content. In general, studies have assessed the usability and user experience of VR prototypes to validate their design guidelines and concepts [184, 206, 117, 207, 40]. However, some vital questions remain unanswered on the wider scale implementation, long-lasting utility and sustainability of these digital products: What are the driving factors behind students' intention to use them? What can prevent students from using them?

How can we assess students in these environments? To our knowledge, no study has directly attempted to answer these questions.

Identification of the underlying human factors in the acceptance of new technology has been a hot topic [208]. Theoretical frameworks on technology acceptance support researchers to hypothesize and investigate various content and context with technology. The Technology Acceptance Model (TAM) [209] and the Unified Theory of Acceptance and Use of Technology (UTAUT) [210] are prominent conceptual frameworks to investigate intended technology use. Meanwhile, several immersive virtual environments with CFD simulations have come out in recent years such as blood flow in cerebral aneurysms [178], farmer education on indoor air quality [37], fire emergency evacuation scenarios [211], communicating the design of modular buildings [181], medical surgery planning [180], as well as automated intelligent systems in industry 4.0 [59]. Unlike other domains, individuals' intention to use such applications has been overlooked most probably due to the complexity of the topic.

6.1.1 Study objectives

In a previous study, we developed the Virtual Garage concept, which is a holistic immersive virtual reality experience to educate students through real-life engineering problems solved with CFD simulation data [207]. We performed a user study to evaluate usability, user experience, task load and simulator sickness while validating applied pedagogical and technological design guidelines. This enabled us to reach an optimized version of the Virtual Garage, in which students can adequately perform tasks and learn without being interrupted by custom design aspects.

As a follow-up to the previous investigation, this study focuses on behavioral intention, task performance and learning in the Virtual Garage. More insight into underlying factors behind students' use of the Virtual Garage may impact the development of long-lasting and sustainable educational experiences with VR technology. Our theoretical framework stems from UTAUT2 – the extended version of UTAUT – to investigate technology acceptance in the Virtual Garage. In addition, learning gain and task performance are also evaluated to elaborate further on the utility of the Virtual Garage in the student assessment. The main objectives of our work are:

- to examine the effect of the UTAUT2 constructs on students' behavioral intention to use the Virtual Garage application,
- to examine users' perceptions and attitudes before and after the use of the Virtual Garage,

- to examine knowledge gain and task performance to develop a summative assessment methodology.

6.2 Research model

6.2.1 UTAUT2: an extended framework

Technology is ever-evolving, and so is technology acceptance of individuals. Various new devices and services are being perennially released to the market aiming at fast and long-term user adaptation. Despite this, it is not always trivial to truly anticipate users' behavior to use and adapt to new technologies. Hence, both academia and industry have developed custom methodologies and performed user studies to uncover significant factors behind individuals' technology acceptance.

TAM was one of the very first models to comprehend users' technology acceptance based on perceived ease of use, perceived usefulness, attitude and behavioral intention [209]. However, the model falls short to truly explaining technology acceptance due to obscured human factors [208]. Advances in user technology have forced the theoretical frameworks to evolve and consider more inclusive and malleable models. One example of this is the UTAUT model, which is made of the eight most substantial acceptance models to assess technology acceptance in workplaces [210]. Technology being a part of daily life, UTAUT was also extended to UTAUT2 by considering the use of technology in a consumer context [212]. A growing body of literature has utilized UTAUT2 to hypothesize and validate the conceptual models on individuals' technology acceptance [208]. The baseline version of UTAUT2 incorporates performance expectancy (PE), effort expectancy (EE), social influence (SI), facilitating conditions (FC), hedonic motivation (HM), price value (PV), and habit (H) as executing factors to determine technology acceptance [212]. UTAUT2 has evidenced its utility to predict technology acceptance, showing that the model achieved some 74% of the coefficient of determination in the behavioral intention of use of new technology [212].

6.2.2 Conceptual model and hypotheses

The ultimate focus of our study is to measure students' behavioral intention to use the Virtual Garage in educational practices. In particular, the Virtual Garage is an immersive learning application blending technology as VR, content as CFD and pedagogy as instructional psychology. Its main goal is to facilitate

an immersive learning environment to reduce the entry barrier for complex engineering concepts and multiphysics CFD simulations, while enabling higher cognitive, affective and behavioral interferences. It appears that the UTAUT2 model is a proven framework to evaluate consumers' behavioral intention concerning fundamental aspects of human factors. In addition, the model has the flexibility to consider external factors to hypothesize technology acceptance concepts in any context. Thus, the model can provide a strong foundation to formulate our hypothesis in the evaluation of the behavioral intention to use the Virtual Garage concept. The conceptualization of the UTAUT model for this particular application was undertaken with regard to the four sets of recommendations given in a recent literature review [208].

First and foremost, we carried out a literature review to identify similar concepts and opt for suitable constructs to explore and examine the behavioral intention of users in the Virtual Garage. Eventually, we structured a conceptual model by incorporating recommendations from the design guideline to structure a model fit better to explore the research context [208]. Fig. 6.1 illustrates our conceptual model composed of original and extended constructs.

We only retained performance expectancy, effort expectancy and behavioral intention from the baseline model. Performance expectancy is defined as the degree of benefits to users in performing certain activities. Effort expectancy is the degree of ease of use. Behavioral intention describes the intentions of an individual to use new technology. Neither social influence nor facilitating conditions were kept in our model since VR technology is not yet widely adopted by institutions or individuals for daily use. Similarly, price value, habit and use behavior were excluded from the model because it is not yet a common personal preference to own VR headsets. Even though VR has recently become commercially affordable, it has not yet been as invasive as other portable user devices.

Hedonic motivation indicates the fun, joy and pleasure that users have during the use of the technology. In our model, we extended hedonic motivation to additionally measure interest, thereby together forming intrinsic value [213]. Literature has shown the importance of interest in similar concepts [214] where users might be potentially interested in either technology or content.

Furthermore, similar to the price that users pay to afford technology, time and effort are imperative resources consumed by users when learning something new. Literature has shown the importance of learning value in technology acceptance in similar concepts [215, 216]. Thus, we incorporated the learning value as a construct in the conceptual model to measure its interrelation with behavioral intention.

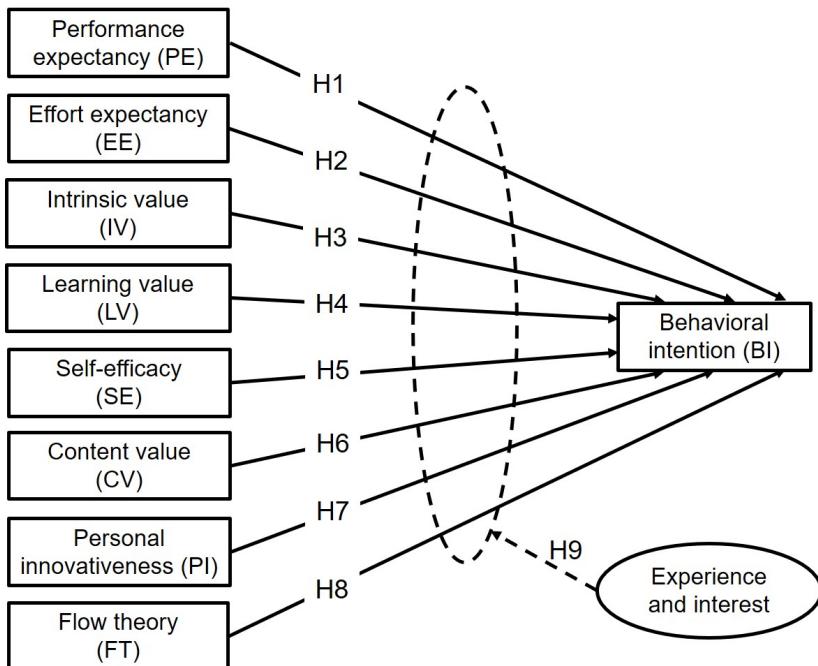


Figure 6.1: The conceptual model in the present study to understand users' behavioral intention in the Virtual Garage.

Users seek content that satisfies their individual preferences. Content is one of the major aspects of individual technology acceptance and use [217, 218, 219, 220, 221]. Users can intend to use a technology or service in order to access the content they are interested in. The content value has become an intriguing parameter in the educational use of VR. Only a limited amount of content for limited contexts are so far made available for students [20]. Therefore, the content value was included in the conceptual framework to better assess the value of educational content.

As mentioned previously, the habit was excluded since users do not own such VR headsets individually. Yet, literature indicated that personal innovativeness may be a triggering factor in technology acceptance. Given the popularity of VR nowadays, innovation-driven individuals may tend to embrace the use of new educational technologies [222, 223]. Researchers have also claimed the positive influence of personal innovativeness on technology acceptance. Eventually, personal innovativeness was incorporated into the conceptual model as a potential predictor of behavioral intention.

In studies utilizing new educational technologies such as smartphones and VR, self-efficacy has been found to be an important predictor of technology acceptance [224, 225, 226, 227]. The construct is mainly formed by competency and belief to tackle a new technology and its operations. Since VR technology has not yet widely been spread among individuals, some users may avoid using it due to lacking competence and belief. Hence, self-efficacy was added to the conceptual model.

The final construct utilized in the extended model is the flow theory, which accounts for users' complete mental involvement in an activity [228]. Perceived enjoyment, perceived control and attention focus, in general, constitute the flow. The theory has also been extended to concentration, immersion, interaction and imagination within the research involving virtual reality [229, 92, 230, 231, 232, 233, 234]. On the whole, the flow theory is a global construct arguably composed of all these constructs and might have a substantial effect on behavioral intention in VR experiences. Our conceptual model was, therefore, expanded with the flow theory including the interaction and immersion as a part of the main construct.

There are also some other constructs that have emerged in the literature but are not adapted to our conceptual model due to their vivid effects on behavioral intention such as simulator sickness. Details are conveyed in the Supplementary information for Chapter 6.

This study examines the behavioral intention of students to use the Virtual Garage application. We propose the following hypotheses:

- H1: Performance expectancy (PE) is a significant positive predictor of behavioral intention.
- H2: Effort expectancy (EE) is a significant positive predictor of behavioral intention.
- H3: Intrinsic value (IV) is a significant positive predictor of behavioral intention.
- H4: Learning value (LV) is a significant positive predictor of behavioral intention.
- H5: Self-efficacy (SE) is a significant positive predictor of behavioral intention.
- H6: Content value (CV) is a significant positive predictor of behavioral intention.
- H7: Personal innovativeness (PI) is a significant positive predictor of behavioral intention.
- H8: Flow theory (FT) is a significant positive predictor of behavioral intention.

Our study moved a step further to examine the moderation effects of interest and experience on behavioral intention:

- H9: Experience and interest in CFD, VR and gaming moderate the relationship between independent constructs and behavioral intention.

6.2.3 Perception and user performance

Aside from the technology acceptance with the UTAUT2 model, pair-wise comparison of some constructs can uncover interesting changes in individuals' perceptions and attitudes toward the technology [235]. Therefore, we decided to evaluate five out of nine constructs in the conceptual model that users can readily rate their perceptions without having used the Virtual Garage: performance expectancy, effort expectancy, intrinsic value, self-efficacy and immersion. We collected users' feedback on these constructs before and after the VR experience.

Furthermore, the increasing popularity of VR in education has convinced some researchers to assess knowledge gain and evaluate learning outcomes. Recent evidence reveals that VR can enhance learning, sometimes even better than traditional practices [6, 190, 20]. Even though in the previous study we conveyed some insights on the assessment of learning in the Virtual Garage [207], we did not provide a structured methodology on how to perform the assessment. Therefore, in this study, as the initial attempt to assess students in the Virtual Garage concept, a summative evaluation approach was developed blending learning gain and task performance.

6.3 Materials and method

6.3.1 VR setup

The Virtual Garage concept is a holistic immersive virtual reality learning experience to educate students through real-life engineering problems solved with CFD simulation data. Technological and pedagogical design guidelines were purposefully applied to benefit the evidence-based workflows. The Virtual Garage is made of two modules; Module#1 and Module#2. The prior aims at teaching VR controllers and the theory of the content with learning tasks. The latter is the assessment where users solve the problem by using CFD simulations. Each module is designed to take 20 min on average with a 5 min break between subsequent modules by taking VR headsets off to mitigate the potency of

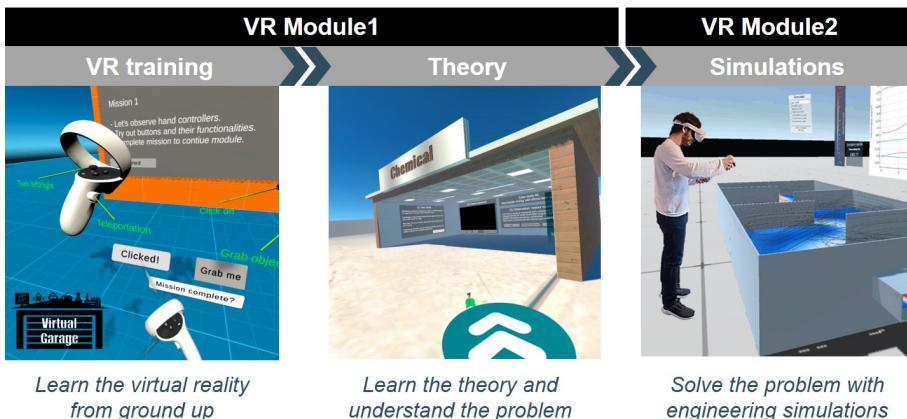


Figure 6.2: Scenes from the modules of the Virtual Garage.

simulator sickness. Users navigate and interact in the virtual environment with teleportation using hand controllers, guided by a laser beam to indicate the exact location. Upon preference, users can choose to be either seated or standing in a confined physical zone. Details on the Virtual Garage concept are available in a previous study [207]. The Unity game engine was utilized with additional packages to develop the VR software. Simulations were run in a workstation by COMSOL v5.6 and integrated by using an extract-based data processing approach [168]. Meta Quest 2 VR headsets were employed to deploy the Virtual Garage.

In this study, we aimed at exploring students' behavioral intention to use the Virtual Garage application together with perception and user performance. In this version of the Virtual Garage as shown in Fig. 6.2, students were expected to learn the fundamentals of the water chlorination process, and subsequently design and analyze a water treatment basin using available CFD simulations. They were supposed to make a decision on a set of parameters to obtain an optimal design that satisfies the design constraints. More information about CFD simulations, verification & validation and learning objectives of the Case#5 study can be found in the Supplementary information for Chapter 6. A walkthrough video and VR software of Case#5 are freely available on YouTube and GitHub, respectively (See the Supplementary information for Chapter 6 for weblinks).

6.3.2 Measures

Empirical data was gathered before, during and after the VR experiments. The pre-tests covered three separate sections: the socio-demographic background of the respondents including interest and experience, the pre-knowledge test, and a part of UTAUT2 constructs to apprehend the effect of perception. Besides, users' activities in the VR were logged to assess their performance by means of time, achievements and decisions. Finally, UTAUT2 and post-knowledge tests were filled by users.

Face validity checks were carried out by researchers in the field to assure that the questionnaire measure the intended knowledge. Subsequently, pilot studies were conducted with postgraduate chemical engineering students to check for misconceptions in the formulation of the questions. Changes were made based on feedback and corrections received. The following sections detail the final version of the items in the questionnaire. We implemented a quantitative methodology to collect, interpret and assess measured metrics to achieve the abovementioned research objectives.

UTAUT2 constructs and items

Items from the baseline UTAUT2 models and available literature were utilized to ensure content validity, thereby compiling a questionnaire to adequately measure intended constructs. The research model contains multiple items for each construct. Items were slightly reworded to make a better fit for the research context. Each item was measured with a seven-point Likert scale, ranging from strongly disagree (1) to strongly agree (7). Items of performance expectancy, effort expectancy and behavioral intention were adopted from Venkatesh et al. (2012). For other constructs, we employed available items in the literature to gather reliable data. The full list of items utilized in this study can be found in the Supplementary information for Chapter 6.

Summative assessment

Knowledge gain and task performance constituted the summative assessments to provide an overall evaluation of students' success. A knowledge test with eight multiple-choice questions was designed to measure knowledge gain based on pre- and post-tests. It consists of items measuring domain knowledge gained through the learning modules and assessing lower and higher cognitive skills in Bloom's taxonomy [67]. Three choices were provided in each question with one correct answer and two credible distractors. The test was validated by peer

chemical engineers. The test is available in the Supplementary information for Chapter 6. Likewise, users' actions in VR were automatically logged and utilized to quantify users' task performance such as total time spent to complete tasks, achievements and decisions.

6.3.3 Participants and recruitment

In order to determine the required sample size, we pursued the advice given by PLS-SEM experts [236]. Checking on Cohen's table for sampling size, the sample size of 54 appeared to achieve a statistical power of 80% for detecting R^2 values of at least 0.25 with a 5% probability of error. Therefore, we aimed at having at least more than 55 participants to make our analysis statistically sound.

Before recruiting participants and conducting the test, an ethical approval (G-2021-4281-R3(AMD)) was received from the ethics committee at KU Leuven to comply with standards for the processing of personal data in academic contexts. The testing was carried out with 57 participants from KU Leuven (Belgium), the von Karman Institute for Fluid Dynamics (Belgium) and Kompetenzzentrum Virtual Engineering Rhein-Neckar Hochschule Mannheim (Germany). A convenience sampling method was intended to reach the target cohort of students from relevant disciplines such as chemical, mechanical and civil engineering.

6.3.4 Data collection and procedure

Experiments were performed in May and June 2022. National and regional safety measures with regard to COVID-19 were applied during the experiments such as proper ventilation of the testing environment, disinfection of equipment and social distancing. Due to the availability of three VR headsets, participants were able to simultaneously participate in the testing. No incentives were provided. Only volunteers joined in the testing.

Testing started with brief instructions on research, ethics, the Virtual Garage application and intended learning objectives. A consent form was signed by participants giving further details on their voluntary participation, experimental procedure, data collection, potential risks and discomforts, anonymity and confidentiality. A paper-pen data collection was carried out for pre- and post-tests. The collected data was digitalized by the researcher. Before the VR experience, users filled in the sociodemographic questionnaire and pre-knowledge test in addition to a portion of UTAUT2 to measure the perception of different

constructs. Users' actions in VR were logged in the VR headsets with the anonymous identities input by users. After the VR experience, users filled post-knowledge test and UTAUT2. Each session took 90 min on average.

6.3.5 Data analysis

Before running the data analysis, the collected data were screened to detect missing and duplicated data. One participant was identified as an outlier by the interquartile rule for outliers. We kept this set of data in the collection since it may be a legitimate part of the population. To justify this decision, we run an exploratory study excluding the outlier from the dataset and compared results to the entire dataset including the outlier. Exploratory study showed that outlier had no significant effect on obtained results. The following sections provide details on the analysis of UTAUT2 analysis and relevant statistical methods to analyze the perception and user performance.

PLS-SEM for UTAUT2

Partial Least Squares Structural Equation Modeling (PLS-SEM) is the most common model to analyze UTAUT2 results as a multivariate analysis method. In this study, we therefore performed the data analysis according to the methodology of Hair et al. [236]. UTAUT2 model was analyzed utilizing a two-step approach as being the most commonly applied methodology in the literature. The first step is the measurement model to conform relationships among items in constructs to sustain reliability and validity by convergent reliability, internal consistency reliability and discriminant validity. The second step is the structural model to create composite models and estimate complex cause-effect relationships in path models with constructs via coefficients of determination, predictive relevance, size and significance of path coefficients, and effect sizes. We employed SmartPLS software to perform PLS-SEM for the conceptual model.

Measurement model

The measurement model assesses whether the relationships among items in constructs are reliable and valid. Once the measurement model is approved, we can proceed with the structural model to predict and analyze technology acceptance.

First, convergent validity is measured to establish a positive correlation between items of the same construct. The items should either converge or share a high proportion of variance. The convergent validity is composed of outer

loadings, indicator reliability and average variance extracted (AVE). To establish convergent validity, outer loadings should be equal to or above 0.708. Indicator reliability is the size of outer loading which is the square of its value and should be higher than 0.5. The AVE value should be or above 0.50 to verify that the construct explains more than half of the variance of its indicators. The guideline demonstrates several examples in case the items do not satisfy the above criteria to maintain convergent validity.

Another metric is the internal consistency to examine inter-correlations between different items to provide a consistent measure for the constructs. Cronbach's alpha and composite reliability are approaches to explain the characteristics of internal consistency reliability. Both should be higher than 0.7 whereas above 0.6 still qualifies for exploratory purposes. While Cronbach's alpha may result in relatively low reliability values, composite reliability can overpredict the reliability. Therefore, it is reasonable to consider and report both criteria, representing the lower level with Cronbach's alpha and the upper level with composite reliability.

Discriminant validity is the final metric assessing whether a construct significantly differs from other measured constructs. It is imperative to maintain discriminant validity to prevent overlapping constructs to measure an indigenous characteristic. Even though cross-loadings and the Fornell-Larcker criterion for discriminant validity assessment have long been traditionally applied by researchers, recent literature does not find these assessments reliable to identify discriminant validity. Instead, the Heterotrait-Monotrait Ratio (HTMT) of the correlations was proposed to carry out a reliable assessment. It can truly indicate the potency of the correlation between two constructs. Running the bootstrapping procedure to derive a distribution of the HTMT statistic, a reliable statistical comparison can be performed to assess discriminant validity. The confidence interval of the HTMT statistic should be lower than 1.

Structural model

Having the measurement model approved, the structural model can be processed to create composite models and estimate complex cause-effect relationships in path models with constructs, thereby evaluating our conceptual models and hypotheses. PLS-SEM was performed to evaluate the structural model and determine path coefficients together with statistical significances, interrelationships and predictions. We used bootstrapping to assess the significance of path coefficients with 5000 bootstrap samples.

First, collinearity is checked to verify that constructs do not have critical levels of collinearity among each other. The construct's tolerance value, namely VIF, should be between 0.2 and 5 to eliminate collinearity, thus eradicating biased

measurements among constructs.

Ensured that the collinearity does not exist, we can run the PLS-SEM algorithm to calculate the structural model and path coefficients to test hypotheses. The path coefficients vary between -1 and +1 for the strong negative and positive relationships in the model, respectively. Path coefficients above 0.2 are in general assumed to have a significant relationship, whereas below 0.1 is insignificant. The relationships become weaker when the path coefficient is close to 0. Furthermore, to detect statistical significance, the bootstrapping procedure is undertaken by calculating t-values, p-values and bootstrap confidence intervals for path coefficients given the context of standardized errors. These three metrics should be utilized to interpret the statistical significance of the path coefficients. Critical values for the metrics are given together with the results.

The coefficient of determination (R^2) is utilized to evaluate the structural model to measure a specific endogenous construct's actual and predicted values such as behavioral intention in our model. The value of R^2 varies between 0 and 1. The higher the value gets, the more accurate the predictive power becomes. R^2 values of 0.75, 0.50 and 0.25 for endogenous latent variables can be respectively described as substantial, moderate, or weak. The effect size of R^2 is determined via the effect size F^2 . It is calculated by omitting a specified exogenous construct from the model and recalculating the R^2 value without the omitted construct. The critical values for F^2 are 0.02, 0.15 and 0.35, respectively, representing small, medium, and large effects of the exogenous latent variable. No effect is assumed below 0.02.

Statistical analysis

Both descriptive and inferential statistics were considered to explore the significance and predict relations among datasets. We employed the R programming language for statistical calculations. The descriptive analysis was run to determine the mean (M), median (MD) and standard deviation (SD), thus summarizing the characteristics of the datasets. Predictions were performed with the applied methods from the inferential statistics. The central limit theorem and normal distribution were checked with the Shapiro-Wilk test. Pre- and post-tests of the perception and knowledge gain were compared using a dependent test for paired samples. For the normally distributed datasets, we utilized the paired samples t-test while the Wilcoxon Signed-rank test was performed for the non-normal distributions. Correlations were applied to increase our understanding of relations in the assessed metrics. Pearson and Spearman's correlations were carried out for parametric and non-parametric

Table 6.1: Sociodemographic information of participants (n=57). *Note: aerospace, water resource, industrial, civil and process engineering. **Note: physics, chemistry, mathematics, biotechnology, bioinformatics and data science.

Characteristics	Items	Frequency	Percentage
Gender	Male	42	73.7
	Female	14	24.6
	No preference	1	1.8
Age	21-23	13	22.8
	24-26	18	31.6
	27-29	15	26.3
	≥ 30	11	19.3
Current education enrolled	Bachelor	9	15.8
	Master	17	29.8
	Doctoral	31	54.4
Discipline	Chemical engineering	24	42.1
	Mechanical engineering	10	17.5
	Other engineering disciplines*	14	24.6
	Others disciplines**	9	15.8

analysis, respectively. Statistical significance was achieved for the p-value < 0.05, which is indicated by a bold asterisk (*).

6.4 Results and discussion

6.4.1 Participant profile

57 participants successfully completed the testing. Table 6.1 illustrates the socio-demographic profile of the participants. The majority of participants were between 24 and 26 years old (31.6%). 54.4% percent of participants were conducting doctoral research, whereas 15.8% and 29.8% were enrolled in bachelor's and master's programs, respectively. Chemical engineering constituted the main training discipline for 42% of the participants and followed by mechanical engineers (17.5%).

Participants also rated their interest, experience and habit in VR, CFD and gaming. Details are available in the Supplementary information for Chapter 6. In brief, approximately 89% of participants were interested in VR, 72% in CFD

and 63% in digital games. 61% and 82% of the participants were novices to CFD and VR, respectively. Speaking of habits, 28% of the participants reported playing games often or more. Interestingly, desktop settings to visualize 3D data were found at least often difficult for some 30% of participants.

Overall, the socio-demographic analysis indicated that the sampled participants can be representative of the target audience for the system in this study, arguably a heterogenous distribution barring gender. Also, interest, experience and habit illustrated the diversity of the population in which participants are in general novices to VR and CFD. Likewise, one of the ultimate goals of the Virtual Garage concept is to enable an immersive visualization environment to help students build spatial reasoning skills. When participants were questioned about the difficulties of desktop setting to visualize 3D data, the overall response was quite high, thus confirming the significance of the Virtual Garage's objectives.

6.4.2 Conceptual model: behavioral intention with UTAUT2

Details on the data analysis of the UTAUT2 model were elaborated in the section 6.3.5. Therefore, in this section, we only presented interpreted and discussed the obtained results. First, we examined the measurement model to verify and validate reliable relationships among items in constructs. Then, the structural model was analyzed to create composite models and estimate complex cause-effect relationships in path models with constructs, thereby evaluating our conceptual models and hypotheses.

Measurement model

Table 6.2 summarizes the assessment of the measurement model. Results showed that the measurement model established a reliable and valid methodology to calculate each construct. Measurements adequately complied with all critical thresholds with satisfying convergent reliability, internal consistency reliability and discriminant validity. Detailed HTMT confidence intervals are available in the Supplementary information for Chapter 6.

Neither items nor constructs exceeded critical values, thus confirming the applicability of the structural model. Results indicated the importance of adapting the intended construct from the available literature to correctly measure the constructs with relevant items. As anticipated, behavioral intention, effort expectancy and performance expectancy constructs from the baseline UTAUT2 model resulted in higher overall scores to validate the measurement model than other constructs. Several external constructs were adopted from the literature

Table 6.2: Summary of the measurement model. All latent variables satisfied the discriminant validity based on the HTMT confidence interval.

Latent variable	Convergent validity		Internal consistency reliability		
	Loadings	Indicator reliability	AVE	Composite reliability	Cronbach's alpha
	0.70	0.50	0.50	0.6	0.6
BI	BI1	0.950	0.903		
	BI2	0.901	0.813	0.848	0.943
	BI3	0.910	0.828		0.910
CV	CV1	0.741	0.549		
	CV2	0.837	0.701	0.623	0.832
	CV3	0.788	0.620		0.697
EE	EE1	0.884	0.782		
	EE2	0.900	0.810		
	EE3	0.877	0.769	0.774	0.932
	EE4	0.858	0.736		0.903
FT	FT1	0.753	0.568		
	FT2	0.738	0.545		
	FT3	0.793	0.628	0.605	0.884
	FT4	0.759	0.576		
	FT5	0.841	0.708		0.838
IV	IV1	0.837	0.700		
	IV2	0.818	0.668		
	IV3	0.733	0.538	0.607	0.860
	IV4	0.722	0.521		0.785
LV	LV1	0.902	0.813		
	LV2	0.932	0.869	0.826	0.934
	LV3	0.892	0.795		0.894
PE	PE1	0.873	0.762		
	PE2	0.889	0.790		
	PE3	0.786	0.617	0.741	0.919
	PE4	0.891	0.793		0.883
PI	PI1	0.822	0.675		
	PI2	0.825	0.680		
	PI3	0.851	0.724	0.704	0.905
	PI4	0.858	0.736		0.860
SE	SE1	0.877	0.769		
	SE2	0.880	0.775	0.774	0.911
	SE3	0.882	0.778		0.861

to build a conceptual model that fits the research context. Learning value, personal innovativeness and self-efficacy revealed good results. Likewise, even though relatively lower than other constructs, content value, intrinsic value and flow theory also scored sufficiently to validate the entire measurement model. It is noteworthy that in the literature flow theory has a malleable form and has been structured in various ways to assess the flow in technology acceptance. In our study, the flow theory construct is constituted by attention focus, interaction and immersion utilizing items from similar but different constructs. Measurement evaluation highlighted that the formed flow theory is a valid and reliable construct.

Descriptive statistics of the constructs are illustrated in Table 6.3 together with percent differences against the highest score. All constructs showed a mean score higher than 5.6, meaning that the results lie between slightly agree and agree but mostly close to agreeing. The intrinsic value and personal innovativeness constructs showed the highest scores, which can be due to voluntarily recruited participants. In contrast, the learning value revealed the lowest score which may be attributed to the participant profile being a novice to technical content, CFD and VR. Participants relatively scored high on the effort expectancy, indicating the easiness of the Virtual Garage to operate and become skillful in VR. The flow theory was also ranked high meaning that participants remained positive toward focus attention, immersion and interaction triggered in the Virtual Garage concept. The content value, self-efficacy, behavioral intention and performance expectancy also resulted in relatively high scores, confirming the importance of content, individual's belief in their capacity to operate VR, enthusiasm toward adopting the Virtual Garage concept and usefulness of the Virtual Garage concept, respectively. All in all, it appears that students show higher likeliness on intrinsic, engaging and enjoyable aspects of the Virtual Garage. This concurs well with earlier findings [204].

Structural model

The structural model was first evaluated without moderating factors. To assess the significance of interest and experience, moderator effects were separately analyzed. The following sections first present and discuss the results of the conceptual model excluding moderators. Then, we elaborate on further investigations on how moderators affected the interrelations among constructors.

Without moderators

Before diving into the structural model, we examined the collinearity to mitigate the effects of bias between constructs. The construct's tolerance value (VIF)

Table 6.3: Descriptive statistics of each construct with mean (M) values, standard deviations (SD), and relative differences against the highest scored construct. The constructs are scored via a Likert scale; 1 (strongly disagree), 2 (disagree), 3 (slightly disagree), 4 (neutral), 5 (slightly agree), 6 (agree) and 7 (strongly agree).

Construct	M	SD	Diff (%)
Intrinsic value (IV)	6.03	0.95	-
Personal innovativeness (PI)	5.98	1.03	0.73
Effort expectancy (EE)	5.93	1.00	1.53
Flow theory (FT)	5.92	0.89	1.83
Content value (CV)	5.89	0.87	2.18
Self-efficacy (SE)	5.81	1.23	3.64
Behavioral intention (BI)	5.71	1.17	5.29
Performance expectancy (PE)	5.69	1.21	5.53
Learning value (LV)	5.64	1.04	6.45

was lower than 5 in all items, thus eliminating collinearity as aimed. The VIF values are available in the Supplementary information for Chapter 6.

Fig. 6.3 demonstrates the conceptual model path coefficient computed by PLS-SEM. The analysis revealed that UTAUT2 can explain influencing factors behind students' behavioral intention to use the Virtual Garage. Table 6.4 summarizes the path coefficients with relevant metrics to interpret the statistical significance.

The learning value was the strongest predictor of students' behavioral intention, indicating that users who find the Virtual Garage concept has value in their learning are more likely to intend to use it. Similarly, the content value showed a significant effect on behavioral intention, meaning that users who find the content in the Virtual Garage concept attractive, useful and understandable are likely to intend to use it. In the previous section, results showed that students overall scored higher likeliness on constructs relevant to engagement, motivation and easy-to-use. In contrast to this finding, PLS-SEM analysis showed that the significant effects behind the students' intention to use the Virtual Garage were the learning value and content value. Due care must be exercised when interpreting mean construct scores and PLS-SEM analysis at the same time. Liking and behavioral intention to use has shown debatable outcomes in different contexts [237, 238]. Our findings showed that there was no noteworthy relationship between liking and behavioral intention to use the Virtual Garage. Recent research argued that the same can also apply in the

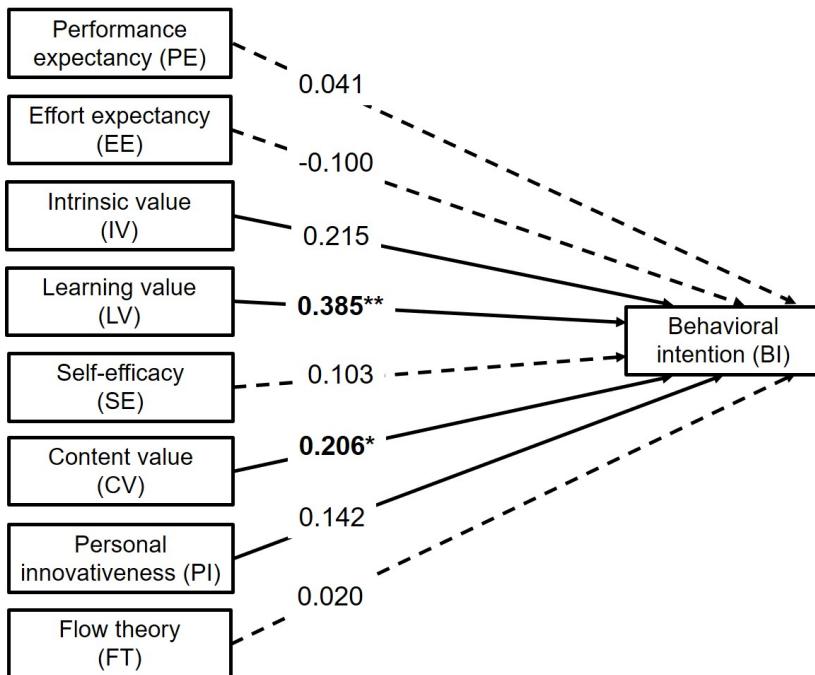


Figure 6.3: Conceptual model with path coefficients. Bold continuous lines indicate important path coefficients bigger than 0.1, whereas level of statistical significance marked by bold asterisks; * for $p < 0.05$ and ** for $p < 0.01$. Dashed lines show no influence of constructs on the BI.

context of learning in immersive technologies: "liking is not learning" [239]. It should be noted that overall learning in immersive technologies can be as effective as traditional practices [240].

Furthermore, intrinsic value and personal innovativeness had positive effects on behavioral intention, even though both brought no statistical significance. These were two constructs that participants rated the highest likeliness. Hence, this likeliness on intrinsic value and personal innovativeness was still positively but insignificantly reflected in the behavioral intention. The learning value and content value are the main driving constructs to convince students to use the Virtual Garage. The results point to the probability that intrinsic value and personal innovativeness can also contribute to the behavioral intention to reach out to more diverse populations. Performance expectancy, effort expectancy, self-efficacy and flow theory showed no effects nor significance on the behavioral

Table 6.4: Constructs with path coefficients, descriptive statistics and statistical significance. Important and significant values are bolded. Critical t-values: 1.28 (significance level = 10%), 1.65 (significance level = 5%), and 2.33 (significance level = 1%). Critical p-values: 0.10 (significance level = 10%), 0.05 (significance level = 5%), or 0.01 (significance level = 1), where level of statistical significance marked by bold asterisks; * for $p < 0.05$ and ** for $p < 0.01$. The path coefficient is significant in case the bootstrap confidence intervals do not include zero,

Construct	Path coefficient (BI)	M	SD	t-value	p-value	Confidence Intervals	
						Bias	Corrected (bootstrap)
						0.05	0.95
CV	0.206	0.202	0.110	1.869	0.031*	0.013	0.371
EE	-0.100	-0.071	0.192	0.519	0.302	-0.362	0.268
FT	0.020	0.027	0.112	0.174	0.431	-0.154	0.210
IV	0.215	0.192	0.157	1.371	0.085	-0.058	0.452
LV	0.385	0.382	0.126	3.047	0.001**	0.170	0.580
PE	0.041	0.058	0.144	0.282	0.389	-0.173	0.297
PI	0.142	0.154	0.123	1.155	0.124	-0.048	0.351
SE	0.103	0.083	0.171	0.604	0.273	-0.214	0.351

intention.

Moreover, the coefficient of determination R^2 was calculated by PLS-SEM to evaluate the predictive capacity of the conceptual model on behavioral intention. Results showed that $R^2 = 0.74$, which corresponds to substantial predictive power on behavioral intention [236]. Table 6.5 shows the effect size F^2 for each omitted exogenous construct. It appeared that the learning value has an impact on behavioral intention more than the medium level. A similar trend emerged in the content value with a small-to-medium effect on behavioral intention. There were small effects of intrinsic value and personal innovativeness observed on behavioral intention. The effect sizes of all constructs were found in line with the path coefficients and statistical significances, thus validating the impact of constructs on behavioral intention.

With moderators

Our analysis of the structural model was extended to examine the effects of moderating factors on behavioral intention. Each moderator was separately inspected to determine its effect between all exogenous constructs and the behavioral intention. Although both positive and negative moderating effects

Table 6.5: The effect size of constructs on behavioral intention. The critical values for f^2 are 0.02 (small effect), 0.15 (medium effect), and 0.35 (large effect), respectively. No effect is assumed below 0.02. Significant effects are bolded.

Omitted construct	Effect size on BI (f^2)	Interpretation of effect size
Content value (CV)	0.0703	small to medium
Effort expectancy (EE)	0.0102	no effect
Flow theory (FT)	0.0006	no effect
Intrinsic value (IV)	0.0411	small
Learning value (LV)	0.1509	above medium
Performance expectancy (PE)	0.0016	no effect
Personal innovativeness (PI)	0.0358	small
Self-efficacy (SE)	0.0139	no effect

were observed on behavioral intention, the results were statistically insignificant. Nevertheless, we identified some interesting patterns to be worth reporting, as summarized in Table 6.6.

Table 6.6: Moderating effects of interest, experience and habit.

Construct	Interest, experience and habit					
	Interested in Gaming	Interested in CFD	Interested in VR	Experienced in CFD	Experienced in VR	Difficult desktop games
CV	-	-	-	-	-	-
EE	0.305 (p = 0.111)	-	-	-	-	0.339 (p = 0.138)
FT	-	-	-	-	-	-
IV	-	-	-	-	-	-
LV	-	-	-	-0.285	-	-
PE	-	-	0.384 (p = 0.104)	0.206 (p = 0.190)	-	-
PI	-	0.204 (p = 0.159)	-	-	-	-
SE	-	0.323 (p = 0.099)	-	0.276 (p = 0.142)	-	-0.223 (p = 0.103)

Effort expectancy with the moderation of the gaming habit positively affected behavioral intention. Interestingly, a similar pattern was also detected with the moderation of interest in the game. The participants who were experienced and interested in digital games found the Virtual Garage easy to use, and this was positively reflected in behavioral intention. It would appear that users' past experience and interest in gaming can lower the entry threshold in terms of usability since users may have been familiar with relevant components from gaming.

Furthermore, the performance expectancy positively affected the behavioral intention within the moderation of the interest in VR. Unlike interest, experience in VR did not show any effect on behavioral intention. Each VR application is composed of custom design elements that diversify the content and overall experience, as well as the level of immersion, interaction and presence. Recent research claimed that the experience with other VR applications may not be a predictor of users' performance concerning simulator sickness [187]. Similarly, in contrast to interest, past experience was not a triggering factor in behavioral intention.

Within the moderation of the interest in CFD, self-efficacy showed a positive effect on behavioral intention. Since participants are interested in the learning content, this may positively alter their attitude and motivation to cope with any issues to prevent them from using the Virtual Garage. Intriguingly, personal innovativeness also became a positive predictor of behavioral intention within the moderation of the interest in CFD. The Virtual Garage is the first of its kind blending CFD simulations with VR as a popular emerging technology. It is very likely that users interested in new technologies and CFD simulations may appreciate the Virtual Garage. It could be thus reasonably assumed that developing interest either in content or in technology prior to the VR experience can convince users to accept the new learning mediums.

Moreover, the moderation of performance expectancy and self-efficacy with the experience in CFD indicated a positive effect on behavioral intention. In contrast to the experience in VR, being experienced in content played a crucial role in behavioral intention. CFD-experienced users demonstrated a higher faith in their performance and beliefs to use the Virtual Garage. This suggests that experience and interest in CFD can have a wider positive effect on behavioral intention than experience and interest in VR. Broadly speaking, the content overtakes the technology when it comes to the moderation of experience and interest. What is surprising is the fact that the experience in CFD moderated a negative relationship between learning value and behavioral intention. Experienced users remained skeptical about learning value and its related factor to the use of the technology. However, this is not particularly surprising in light of the fact that experienced users may seek advanced features to interact with CFD data as

being provided in CFD software for expert users. Instead of performing a whole CFD project, the Virtual Garage aims at facilitating a learning medium where CFD data can be utilized as learning content whilst providing a first contact for non-CFD expert users. CFD simulations have a complex custom workflow that is generally undertaken through an exploratory iterative fashion. Hence, experienced users may find the VR experience limiting, resulting in a negative tendency toward the behavioral intention.

Finally, we assessed the moderating effect of having difficulties visualizing 3D data on desktop settings between constructs and behavioral intention. Results revealed that self-efficacy negatively affected the behavioral intention of this moderation. In other words, it appeared that the ones having difficulties visualizing 3D data on desktop settings reported lower self-efficacy and this negatively affected their behavioral intention to use the Virtual Garage. This result provides valuable evidence for the importance of the competence and self-belief of users in technology. Users already having difficulties with desktop settings pointed out a similar tendency to lack confidence and competence to operate the VR experience regardless of the content. One of the main objectives of the Virtual Garage is to help non-expert users develop spatial reasoning skills to properly interpret CFD simulation data thanks to spatial immersion and advanced interaction in VR. However, either being or feeling incompetent to operate VR experiences might hamper the learning activity and may turn the Virtual Garage into a futile attempt to help in cognition for this portion of users. Therefore, it seems likely that getting users in contact with a generic practicing VR experience prior to the Virtual Garage may increase their competency and belief in VR technology whereas preventing potency of the cognitive overload.

Perception and attitude

Table 6.7 illustrates differences between pre- and post-test scores of measured performance expectancy, effort expectancy, self-efficacy, intrinsic value and immersion constructs. According to the statistical analysis, effort expectancy, self-efficacy and immersion significantly increased after the use of the Virtual Garage, whereas performance expectancy and intrinsic value had no significant changes. Users demonstrated higher perceived ease-of-use (effort expectancy), competency and belief to operate VR (self-efficacy), and immersion after being exposed to the Virtual Garage. Results indicated the importance of prior experience in technology and content. While the prior experience can encourage users to properly operate VR applications, it can also help them truly apprehend the immersion confirming previous findings [235]. It is noteworthy that several technology acceptance studies are available in the literature solely measuring the perception without any active interaction of the users within the actual

digital content. Although the goal was in general to only measure the technology acceptance based on the initial perception, it may result in weak and misleading argumentations, thus diverting and hindering the underlying factors.

A correlation analysis was performed to further explore how post-tests of five constructs were related to individuals' interests and experiences as utilized in the moderation analysis. Since the dataset is not normally distributed, we used Spearman's correlation. We only report detected correlations. Interest in VR positively correlated to performance expectancy (**p = 0.015***, r = 0.319) and effort expectancy (**p = 0.019***, r = 0.310), whereas experience in VR only positively correlated to performance expectancy (**p = 0.038***, r = 0.274). Results indicated that the ones interested and experienced in VR showed a positive attitude toward performing better in the Virtual Garage. This substantiates the positive moderating effect of the interest in VR between performance expectancy and behavioral intention as previously discussed. In addition, interest in gaming positively correlated to performance expectancy (**p = 0.036***, r = 0.277), effort expectancy (**p = 0.020***, r = 0.306) and self-efficacy (**p = 0.012***, r = 0.330). Users interested in gaming reported better performance, ease of use, competence and self-belief to operate the Virtual Garage. Likewise, interest in CFD positively correlated to intrinsic value (**p = 0.015***, r = 0.319). As expected, an intrinsic intention was observed in the CFD-interested portion of the participants. It would seem that users' intrinsic motivation and interest can be triggered by having the digital content they are interested in.

Table 6.7: Change in perception and attitude. The level of statistical significance marked by bold asterisks; * for $p < 0.05$ and ** for $p < 0.01$.

Construct	Performance expectancy		Effort expectancy		Intrinsic value		Self-efficacy		Immersion	
	Pre	Post	Pre	Post	Pre	Post	Pre	Post	Pre	Post
Mean	5.88	5.69	5.39	5.93	5.99	6.03	5.30	5.86	5.57	6.05
Change (%)	-3.13		10.09		0.59		10.68		8.66	
Wilcoxon	$V = 613.5$		$V = 230.5$		$V = 431$		$V = 195$		$V = 99$	
Signed-rank test	$p = 0.2792$		$p = 0.0002**$		$p = 0.8011$		$p = 0.000004**$		$p = 0.00035**$	

6.4.3 Learning and task performance

In this research, we further made an effort to observe the effect of the Virtual Garage on knowledge gain and task performance. We initiated a custom summative assessment as a preliminary work toward integrating an assessment methodology in the Virtual Garage.

Knowledge test

Knowledge gain was composed of 12 multiple-choice questions in which each correct answer scored 1, with 12 as the maximum total. Descriptive statistics showed that there was a 17.1% increase in the mean score of post-test ($M = 8$, $SD = 1.71$) in comparison with the pre-test ($M = 6.63$, $SD = 1.94$). Statistical significance was assessed with a pair-wise analysis by comparing mean values of pre- and post-test scores. Shapiro-Wilk normality test showed that a non-parametric analysis should be applied to analyze the chance between pre- ($W = 0.965$, $p = 0.105$) and post-tests ($W = 0.911$, $p = 0.0005$). Since the dataset is not normally distributed, we used the Wilcoxon signed-rank test. The test showed a significant statistical increase between pre- and post-tests ($V = 174$, $p = \textbf{0.00002}^{**}$), indicating that students significantly performed better in the post-test. No significant correlation was detected between learning and interest & experience.

Task performance

Users' actions in the Virtual Garage were collected to form an assessment methodology including logged metrics. Exposure time and decisions were logged. The Virtual Garage has two subsequent modules of 20 min with a 5 min break in between to prevent long exposure time and to reduce simulator sickness. Users on average spent 19.5 min ($MD = 18.9$, $SD = 4.7$) and 13.8 min ($MD = 15.5$, $SD = 5$) in Module#1 and Module#2, respectively. Time was not included in the assessment since it is not a metric measuring individual's success in the Virtual Garage concept.

Task performance was assessed with final decisions made by users in Module#2. At the end of Module#2, users filled in a decision-making board to provide a final design that satisfies the given constraints. Table 6.8 summarizes overall scores and percentage distributions in the population. According to Spearman's rank correlation, we detected a positive correlation between the post-knowledge test and task performance ($p = \textbf{0.022}^*$, $r = 0.301$). No correlation was

Table 6.8: Scores of post-knowledge test, task performance and summative assessment.

Test	Percent distribution of test scores (%)				
	0-19	20-39	40-59	60-79	80-100
Post-knowledge	0.0	5.3	26.3	50.9	17.5
Task performance	33.3	3.5	12.3	7.0	43.9
Summative assessment	1.8	35.1	10.5	10.5	42.1

revealed between task performance and experience & interest and perception, thus matching earlier findings [241].

Summative assessment

We developed a summative assessment methodology in which the final score is made up of 50% learning gain and 50% task performance. More on the summative assessments can be found in the Supplementary information for Chapter 6. Table 6.8 presents the entire scores in the context of the summative assessment. No significant correlation was found between the summative assessment score and UTAUT2 constructs, as well as experience & interest.

We believe that the assessment methodology should be customized based on the utility of the Virtual Garage concept. On the one hand, if practitioners solely look for an edutainment tool, they can either use an online questionnaire or carry out an interview session to get some insights and reflections on students' experiences instead of learning outcomes. On the other hand, as utilized in our work, an assessment methodology can be developed and implemented in the relevant courses and exercises.

An assessment rubric with intended learning outcomes may help lecturers come up with a fair evaluation scheme. We advise lecturers to progressively implement similar applications in educational practices since several unknown aspects of assessment might appear along the journey. For example, complementary assessment tools can further be implemented in learning modules to provide a ground for self-evaluation and reflection via the learning analytics dashboards.

6.4.4 Practical implications: limitations and future directions

Instead of performing the experiments in a classroom environment, we recruited participants through a convenience sampling method. Therefore, repeating the experiments within a larger and heterogeneous population from university courses may provide further validation to our findings. Also, the results were mostly based on graduate students, as 84% of the participants were enrolled in a master's program or higher. To truly understand the behavioral intention of younger groups - such as undergraduate students - it would be valuable to perform a follow-up study. Another limitation of our study was the imbalanced gender ratio, as our population was dominated by male participants (73.1%). This prevented us to examine any gender-related aspects. Lastly, we are aware that it is expected to compare the Virtual Garage against available educational practices. However, a traditional version of the Virtual Garage is not available. Hence we did not attempt to perform a comparison study. Instead, as previously proposed [207], it would bring more added value to compare the effect of immersion and other relevant factors such as usability and learning between variants of CFD scenes in VR.

VR technology has a dynamic trait, day by day becoming more affordable, accessible and diverse owing to advances in hardware and software. We, therefore, convey some direction for future works concerning today's situations in technology. First, more research could be concentrated on the practical implementation of VR in a current educational context. Best practices could be properly assessed and reported. Not only students but also lecturers including all other stakeholders would be a part of the implementation and assessment. Secondly, the metaverse is being transformed from hype to reality. Collaborative learning environments, where peer students and lecturers can be simultaneously present, would be an intriguing direction. Lastly, the added value of VR in remote education would be worth studying to figure out the underlying factors behind both students' and decision-makers' behavioral intentions.

6.5 Conclusion

This study explores the underlying factors behind students' behavioral intention to use an immersive virtual reality learning environment with CFD simulations, namely the Virtual Garage concept. Learning value and content values are driving factors in the students' behavioral intention. In other words, it appears that students can continue using similar applications if only it has a learning value with content that matters for their education. Intrinsic value and personal innovativeness also show a positive impact on behavioral intention. We provide

further evidence of the importance of perception. Participants' perception of effort expectancy, self-efficacy and immersion significantly and positively increased after using the Virtual Garage. In addition, considerable progress in the evaluation of learning and performance is also demonstrated. Our results provide encouraging findings for practitioners and decision-makers in the design, development and implementation of similar digital educational tools.

Chapter 7

Conclusion and perspectives

7.1 Extensive conclusion

The general aim of this dissertation was to implement CFD simulations with immersive technologies in engineering education. The study was undertaken in four major steps to achieve this goal. This chapter gives an extensive conclusion on our work.

First, we developed a data processing methodology to integrate CFD data in game engines. Although CFD is a mature and broadly applied engineering tool to solve complex problems in a time cost effective manner, educational use of CFD has been limited due to technical and conceptual challenges to create the intended learning experiences. Immersive technologies, such as AR/VR, can be digital mediums to democratize the educational use of CFD simulations. Despite the many recent attempts, the literature lacked a system development procedure to integrate CFD simulation data into game engines, which are cross-platform tools for building AR/VR software. To date, AR/VR applications with CFD data suffered from platform-specific, computationally-demanding, nonreplicable and manually integrated data processing methodologies. This hindered developers to consider AR/VR tools to visualize CFD simulation data. After an extensive feasibility study, our work initially proposed a component-oriented system architecture. This architecture essentially promotes dedicated workflows to integrate CFD data from commonly utilized CFD software into game engines to build AR/VR applications. This can sufficiently guide non-CFD experts to comprehend the multiplatform integration of CFD data into game engines, as well as to figure

out data processing pipelines in technical development. The study explored the potential of data processing options throughout the preparation of the simulation dataset with AR/VR. We developed an extract-based data processing methodology with lightweight, easy-to-implement, end-to-end, automated and free-to-use utilities. Any kind of digital device, regardless of computational power, can be employed to run AR/VR applications with CFD simulations, as a significant step in the democratization of CFD simulation results. The extract-based data processing methodology was quantitatively and qualitatively assessed to determine adequate data formats concerning data processing size, time and quality. In addition, an automated data coupling strategy was for the first time introduced to ease cross-platform integration from CFD software to game engines. We focused on a rigorous integration methodology that practitioners can readily pursue to develop educational AR/VR environments with CFD simulations. The findings of the present study can help practitioners to integrate desired simulation results with the aid of newly adapted technologies in engineering education.

Secondly, a two-way connected system was structured and assessed to facilitate sustainable immersive applications with CFD simulations. Early research in this field primarily focused on the automation of CFD solvers to produce data for cross-platform environments, rather than two-way coupling. Challenges related to a fully coupled computing system stressed the need for an expert to maintain automated data generation and simulation routines. Therefore, AR/VR applications with CFD simulations mostly remained stand-alone and non-interactive. A remote content delivery model was introduced with a client-server network. The integration is strictly tied to modular, automated, easy-to-update, lightweight, end-to-end and open-source utilities. Any end-user device is made employable regardless of hardware performance using the extract-based data processing model introduced in Chapter 3. Both OpenFOAM and COMSOL are simultaneously connected to the Unity game engine. Seamless integration was prompted between CFD software and user applications to obtain connected, long-lasting and sustainable user applications. Automated workflows are flexible and readily customized for any compelling needs with the modular architecture. The system also highlights practices to develop co-simulation and digital twin environments with interactive CFD simulations that are remotely accessible. The system performance of technical integrity was assessed to ensure a feasible and effective connection through the client-server network concerning data processing, dataflow, data management and delivery systems in the network. We demonstrated a set of human-centric features to interact with CFD simulations in VR. A task-centered educational model was additionally introduced within the case study to design digital learning environments concerning complex skills to be developed by learners to work with CFD simulations.

Third, we developed a VR application to operate an immersive learning experience with CFD simulations. The VR application was evaluated by users to validate the design guidelines utilized in the conceptualization. The cognitive, affective and behavioral advantages of virtual reality (VR) can help lecturers reduce entry barriers to concepts that students struggle with. We introduced the Virtual Garage application as a task-centered educational VR application with CFD simulations. The Virtual Garage is a holistic immersive virtual reality experience to educate students through a real-life engineering problem solved with CFD simulation data. The focal point of our work was to investigate the learning effectiveness together with cognitive, affective and behavioral aspects of immersive learning with CFD simulations. Nonetheless, to perform a reliable evaluation of these metrics, we initially focused on the assessment of the design parameters in the Virtual Garage concept. To validate the design guidelines applied to the Virtual Garage concept, we performed a user study ($n=24$) assessing usability, user experience, task load and simulator sickness with both quantitative and qualitative metrics. Our analysis indicated promising results regarding the design, development and evaluation of CFD simulations in immersive learning. Considerable progress was made with regard to the quality of the immersive learning experience with CFD simulations assessing usability, user experience, task load and simulator sickness. Concerning the scarcity of relevant literature to date, our findings and remarks may help developers to find proper guidance in their development journeys.

Finally, we evaluated behavioral intention and perception, as well as assessed learning and task performance. In Chapter 5, we validated the Virtual Garage concept and additionally identified a set of items to further increase the quality of the digital tool. We accordingly processed these additions and performed a follow-up study. Besides, we explored behavioral intention, perception and user performance in the Virtual Garage recruiting 57 participants from three different institutions. Learning value and content values are driving factors in the students' behavioral intention. In other words, it would appear that students can continue using similar applications only if it has a learning value with the content that matters for their education. Intrinsic value and personal innovativeness also show a positive impact on behavioral intention. We provided further evidence of the importance of perception. Participants' perception of effort expectancy, self-efficacy and immersion are significantly and positively increased after using the Virtual Garage. Moreover, the VR application helps students perform significantly better in the post-knowledge test. Considerable progress on the evaluation of learning and performance was also achieved. Our results provide encouraging findings for practitioners and decision-makers to achieve on-target immersive virtual reality learning environments in higher education.

7.2 Perspectives

In this research, significant progress was made throughout four major steps in the design, development and evaluation of immersive technologies with CFD simulations in engineering education. Despite the accomplishments inherently relying on our research objectives to integrate multiphysics CFD simulations in immersive learning environments, each step posed more questions than we attempted to answer. Our research also yielded questions in need of further investigation. In this section, we look into potential research directions that might lead the way to advanced and sustainable immersive learning environments with CFD simulations.

An extract-based data processing methodology was developed to integrate CFD data into game engines in Chapter 3. We merely utilized data formats officially supported by software incorporated in the data processing workflow. There are newly released data formats available offering lightweight and quality alternatives to existing ones, such as Graphics Language Transmission Format (GLTF). However, CFD software and game engines do not directly give support for GLTF format, which is still based on unreliable custom data processing pipelines. It might be interesting to investigate newly adapted lightweight data formats to reduce data size and increase data processing speed while preserving quality. Further research may keep an eye on new data formats to benefit advanced features as long as they become officially supported by CFD software and game engines. Eventually, this could also result in simpler data processing pipelines.

In Chapter 4, we introduced a client-server architecture to remotely deliver content between the server where all computations are performed on desktop premises and the clients as end-users with immersive devices. In recent years, different conceptual models have been developed to build an inclusive computational ecosystem. Ubiquitous computing has received much attention for decentralizing and distributing computational work using any device from any location in any format. Desktops, smartphones, tablets, wearables, sensors and any other electronic devices can be implemented in ubiquitous computing. Further research regarding the role of ubiquitous computing would be worthwhile to incorporate novel computational concepts into the client-server architecture in support of interactive CFD simulations with immersive technologies. Moreover, a future study investigating real-time CFD simulations in immersive hardware would be also very interesting. Current computational models and immersive hardware have a very limited capacity that can only solve the basics of fluid dynamics toward engineering accuracy. If the target is complex and multiphysics models are involved, a number of possible studies are apparent such as using reduced order models (ROM) and artificial intelligence (AI). CFD

software developers have recently concentrated on ROM and AI to accelerate simulation workflow. Further investigations are needed to understand how accelerated models can be implemented in game engines to enable a real-time CFD simulation tool in immersive environments. Not only education but also industry can exploit this technology in support of a time-cost effective decision-making process, as well as in digital twins and a variety of industry 4.0 products.

The Virtual Garage concept was demonstrated in Chapter 5, which is an immersive virtual reality learning environment to solve real-life engineering problems with CFD simulations. The Virtual Garage is composed of two subsequent modules; Module#1 and Module#2. The former is a procedural learning environment to teach interaction in VR and provide supporting information on content with relatively easy tasks to be completed by users. The latter is an assessment environment mainly comprising data interpretation, problem-solving and decision-making by using pre-computed CFD simulation data. Available pedagogical guidelines, such as multimedia learning and instructional design methodologies, were utilized in the design of learning modules. We performed a comparative evaluation between Module#1 and Module#2 to understand the effect of CFD simulations on usability, user experience, task load and simulator sickness. Further research in this field would be of great help in the design of optimal user interfaces and interaction with CFD data in VR. Throughout a value-added approach, user interfaces with custom design elements can be comparatively examined to figure out optimal features, through which non-experts can effectively interact with and interpret CFD data. Broadly speaking, there may be different needs for user interface and interactions among the applications based on discipline, content and target group – for example medical experts versus chemical engineering students. Moreover, the educational use of VR applications with CFD simulations can be hindered due to individuals' vulnerability to immersive technologies and insufficient infrastructures to accommodate an entire class of students. For such instances, a desktop version of the VR application - such as a computer game - can be built into game engines as an alternative option. It is noteworthy that immersive technology is not immersive learning on its own, but it is a part of immersive learning to leverage the level of immersion, interaction and presence. Although a desktop version can negate the effect of immersion, students can still benefit from the Virtual Garage as being a user-friendly educational digital application with CFD simulations. A further study could compare the desktop and VR versions of the Virtual Garage concept in terms of immersion, interaction and presence, as well as their reflection on cognitive, affective and behavioral domains.

Behavioral intention to use, perception and user performance were studied

within the Virtual Garage concept in Chapter 6. Notably, a methodology was presented and implemented to assess users by combining the learning test and task performance. This was one of the very initial attempts to measure learning and to broaden our scope in the trajectory of educational implementation. Further research regarding the role of learning assessment in VR would be worthwhile since the current literature provides relatively limited guidance to embrace best practices. It would be interesting to start with traditional learning assessments and to progressively incorporate and adopt emerging methods in line with learning objectives and technology such as peer assessment, learning analytics, reflection and communication throughout a student-centered approach. Furthermore, not only students' but also lecturers' behavioral intention to use VR in their teaching practices and perception would be an interesting study to reveal hindering factors behind mass adoption. Investors, decision-makers and policy-makers may well receive these outcomes and act accordingly. More research should be concentrated on the practical implementation of VR in a current educational context. Best practices should be properly assessed and reported. Not only students but also lecturers and all other stakeholders should be a part of the implementation and evaluation.

Immersive technologies are becoming more affordable, accessible and diverse thanks to advances in hardware and software. Therefore, it is substantial to convey some directions for future works concerning today's situations in technology. Remote learning has increasingly become a popular realm. Comparing in-class and remote use of VR and its effect on learning would be a valuable contribution. Likewise, collaborative features may further be an enabler for remote and social learning given the increasing popularity of metaverse-like educational environments whilst incorporating the connectivism in immersive learning. Not only education but also engineering can benefit from the multiplayer option to effectively and collaboratively communicate CFD simulation data in immersive VR. Lastly, in terms of software development and post-production workflow, more structured and user-friendly authoring tools may well encourage practitioners to try and adopt to such digital environments.

Educational use of immersive technologies with CFD simulations is an interdisciplinary topic interfering with applied engineering, computer science and pedagogy. This research has been undertaken in the framework of the European Training Network for Chemical Engineering Immersive Learning (CHARMING) project, in which a strong collaboration has taken place among engineers, educational scientists and game developers. The overall implication of our findings and research in CHARMING project is that an interdisciplinary team is essential to properly structure and undertake such challenging and complex research questions. In addition to this, practicing networking within related associations and communities from both local and international levels,

such as XR4ALL initiation by the European Commission, can be a great opportunity to obtain the required support in every stage of the immersive learning development journey from finding open-source technical tools to participants for user experiments.

Appendix A

Supplementary information for Chapter 3

Table A.1: Details on 3D data formats in computer graphics.

3D data format	Developer	Type	ISO standard	SDK	File type	Web browser integrity	Initial release
3DS	Autodesk Inc.	proprietary	-	+	binary binary	converter	1996
BLENDER	Blender Inc.	neutral	-	-	and ASCII	converter	?
X3D	Web3D consortium	neutral	+	-	binary	converter	2001
FBX	Autodesk Inc.	proprietary	-	+	binary and ASCII	converter	2002
GLTF	Khronos Group	neutral	-	-	binary	direct	2016
OBJ	Wavefront Technologies	proprietary	-	-	ASCII	direct	1990
STL	3D Systems	neutral	-	-	binary and ASCII	converter	1987
STEP	Autodesk Inc.	neutral	+	-	ASCII	converter	1994
DAE	Khronos Group	neutral	+	-	ASCII	converter	2004
WEBGL	Khronos Group	neutral	-	-	-	direct	2017
VTKJS	Kitware	neutral	-	-	-	direct	2017

Table A.2: Data encoding characteristics of 3D data formats.

Data encoding characteristics		3DS	BLENDER	X3D	FBX	GLTF	OBJ	STL	STEP	DAE	WEBGL	VTKJS
Geometry	Approximate mesh	+	+	+	+	+	+	+	+	+	+	+
	Precise mesh	-	+	+	+	+	-	+	+	+	+	+
	Constructive solid	-	+	+	-	-	-	+	-	-	-	-
	geometry											
Appearance	Color	+	+	+	+	+	-	-	+	+	+	+
	Material	+	+	+	+	+	-	-	+	+	+	+
	Texture	+	+	+	+	+	-	-	+	+	+	+
Scene	Camera	+	+	+	+	+	-	-	+	+	+	+
	Light	+	+	+	+	+	-	-	+	+	+	+
	Relative position	+	+	+	+	+	-	-	+	+	+	+
Animation	Animation	-	+	+	+	-	-	-	+	+	+	+

Table A.3: A comparison between CFD software.

CFD software	OpenFOAM	COMSOL	Ansys	Star-CCM+	Numeca	SimScale
Developer	OpenCFD Ltd.	COMSOL Inc.	Ansys Inc.	Siemens	Numeca	SimScale GmbH
Version	v6/2018	v5.4/2018	v18/2017	2019	2019	2019
License	open-source	commercial	commercial	commercial	commercial	commercial
Operation	C++/Python Linux, MS, MAC	Java/Matlab Linux, MS, MAC	C Linux, MS, MAC	Java Linux, MS, MAC	MS, MAC paid	C++ Linux, cloud paid
Parallelization	free	paid	paid	paid	paid	paid
Modeling	CFD Multiphysics	+	+	+	+	+
Database	File vs Management	file-based system	management system	management system	management system	management system
Support	Example models	tutorials application gallery	tutorials	tutorials	-	application gallery

Table A.4: Data import and export options currently provided by CFD software.

	CFD software	OpenFOAM	Consol	Ansys	Star-CCM+
CAD	Import Export			Either external or embedded software with several 3D CAD file formats	
	Import Export			Either external or embedded software to generate suitable mesh file formats	
Mesh	Import Export			ABAQUS, ANSYS CFD-Post, CGNS, EnSight, Fieldview, Tecplot, Nastran	STAR-View+ and VRML
	Import	CPP	Consol and Nastran		
Simulation	Import Export	CPP and txt	mph, mphbin, mphtxt, mphphp, txt, csv, dat, xlsx, Nastran, vtk	CGNS, HDF, XDMF, NetCFD, EnSight, Fieldview, Tecplot, Nastran, ParaView, csv, txt, xml, cdb, dat, case	Fieldview, techplot, sbd, Nastran, CGNS, HDF, csv, txt, xml
	Media file formats Text file formats 3D data formats	- + -		+	+
Post-processing			+ VRML	+ VRML	+

Table A.5: Data import and export options currently provided by CFD post-processors.

Postprocessing software		Ensight	FieldView	Tecplot	ParaView
Operation	Developer	Ansys Inc.	Vela Software International	Vela Software International	Kitware
	Version	2019	2019	2019	2019
	License	commercial	commercial	commercial	open-source
	API	Python	Python	Python	Python/C++/ Java/Web
	Source code manipulation	restricted	restricted	restricted	open-field
	Operating system	Linux/MS/MAC	Linux/MS/MAC	Linux/MS/MAC	Linux/MS/MAC
Post-processing	Image and video file formats	+	+	+	+
	Text file formats	+	+	+	+
	Data exchange with other software			Ansys, OpenFOAM, Comsol, Star-CCM++, Ensight, FieldView, CGNS, HDF, XDMF, NetCFD, VTK and many others	
3D data formats	OBJ, STL, STEP	STL, Parasolids, IGES, Native CAD, XDB	with extension	SVG, GLTF, VRML, X3D, JSON, VTKJS, WEBGL	
	Virtual reality	plugin	plugin	plugin	plugin

Table A.6: 3D computer graphics software for rendering and data processing.

Application	3ds Max	Blender	Houdini	Maya
Developer	Autodesk Inc.	Blender	Side Effects Software	Autodesk Inc.
Version	2019	v8.1/2019	2019	2019
Platforms	MS	MS/MAC/LINUX	MS/MAC/LINUX	MS/MAC/LINUX
License	proprietary	open-source	proprietary	proprietary
Text file	plugin/coding	plugin/coding	plugin/coding	plugin/coding
import/export	FBX, 3DS, PRJ, ABC, AI, DAE, HTR, OBJ, SHP, SKP, STL, TRC, VRML, Openflight FLT, DEM, XML, DDF, DWG, DXF, IGE, IGS, IGES, IPT, WIRE, IAM, LS, VW, LP, SAT, Catia V4/V5, JT, ProE, RVT, PRT, STEP, WIRE	DAE, Alembic, FBX, BVH, PLY, OBJ, STL, SVG, DXF X3D, glTF	-	Maya Ascii, Maya Binary, MEL, FBX, OBJ, STL, Openflight FLT, DXF, IGES, VRML2

Table A.7: A comparison between prominent game engines.

Game engine	Unity 3D	Unreal	Game Maker Studio 2	CryEngine SDK
Developer	Unity	Epic games	Yoyo Game Maker	Crytek
Version/ released date	v2019.1.0/2019	2019	2019	2019
Platform	MS/MAC/LINUX	MS/MAC/LINUX	MS/MAC/LINUX	MS/MAC/LINUX
License	free/paid	free/paid	Proprietary	Proprietary
API	C#, Java	C++	C++	C++, Lua, C#
Image, video, and audio import/export	+	+	+	+
Text file import/export	plugin/coding	plugin/coding	plugin/coding	plugin/coding
3D Data import/export	FBX, DAE, 3DS, DXF, and OBJ	FBX, DAE, 3DS, DXF, and OBJ	plugin	CGF, CGA, MA, ATOM, DAE, ZIO, FBX, ABC, CBC and CAX
AR support SDK	ARKit, ARCore, Vuforia, AR Foundation, Magic Leap, Hololens	ARKit, ARCore, Handheld AR, Magic Leap, Hololens	plugin	PlayFusion
VR support SDK	Stream VR, OpenVR, Vivewave, middle VR, oculus vr, samsung gear	Steam VR, Google VR, Oculus VR, Samsung gear VR, Unreal VR engine	plugin	OSVR

Table A.8: 3D data formats and the support of cross-platforms to integrate CFD data into computer graphics.

Table A.9: Data- and workflow of the development procedure in details from the system architecture.

Component	Data creation						AR/VR technology						Data processing						End-user console														
	CAD	Preprocessing	Stimulation	Post-processing	Database	Extraction	Transformation	Virtuality	Content of immersion	Perception	Integration	Interaction	Android	Windows	Unity	Android	Windows	Unity	Android	Windows	Unity	Android	Windows	Unity	Android	Windows	Unity	Android	Windows	Unity	Android		
System requirements	OS	Windows	Ubuntu	Windows	Windows	Windows	Windows	Windows	Windows	Windows	Windows	Windows	Blender	Windows	Windows	Android	Android	Windows	Android	Windows	Android	Windows	Android	Windows	Android	Windows	Android	Windows	Android	Windows	Android		
System requirements	Software	FreeCAD	OpenFOAM	Paraview	ParaView	File-based	Paraview	Blender	Blender	Unity	Unity	Unity	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia	Vuforia		
System requirements	Hardware	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop	laptop		
System requirements	Addin	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-		
Programming language	Network	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-		
Programming language	IoT	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-		
Data analytics	Dataflow	1	2	3	4	5	6	7	8	9	10	11	12	13	14	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX
Data analytics	Format	STL	FOAM	X3D	OBJ	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	FBX	
Data analytics	Size (MB)	2	122	4807	4807	85	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12
Data analytics	Processing period (s)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
Data coupling	One-way	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	

required packages

Appendix B

Supplementary information for Chapter 4

A video walkthrough of the user experience in the VR environment is available on YouTube: https://www.youtube.com/watch?v=5Khu_bZhtZI.

Codes and packages utilized in this work are freely available on GitHub: <https://github.com/sersolmaz/CFD-CDN-UNITY>.

Appendix C

Supplementary information for Chapter 5

Free access to the VR application and the walkthrough video

The Virtual Garage with Case#6 is freely downloadable on GitHub: <https://github.com/sersolmaz/The-Virtual-Garage>

A walkthrough video of the Case#6 is available on YouTube: https://www.youtube.com/watch?v=Lv__-H10eMY

List of challenges impeding the adoption of VR in engineering education

Recently published reviews have come up with a broad list of challenges that are dramatically impeding adoption of VR in engineering education, summarized as follows:

- lacking reliable guidelines and standards in the design, development and implementation [39, 21];
- difficulties in finding and producing relevant digital content [39, 21];
- missing user-friendly customization and authoring tools [192, 39, 242];
- discouraged novice students and practitioners to adopt the technology [18, 39, 21];
- language barriers [39];

- irrelevant and superficial user evaluation metrics obscuring underlying reasons [13, 20, 39];
- subjective and primitive data analyses [18, 39];
- weakly utilized mixed, qualitative and quantitative methodologies [18, 39];
- missing learning theories and inadequate instructional design methodologies [18, 15];
- undervaluing multidisciplinary collaborations among engineers, educators and software developers [18].

4C/ID and multimedia principles in the Virtual Garage concept

Table C.1 details the implementation of the 4C/ID model in the Virtual Garage concept. The relevant principles are adopted from the original guideline [72]. Overall, several principles of multimedia learning are applied in the components of the 4C/ID model in the Virtual Garage concept. The learning task is structured toward the sequential principle to enable a learning environment to increase the complexity progressively. We also benefit from the variability principle by using a non-linear progression across subtasks due to its positive reflection on better test scores [72]. Besides, the supportive information is shaped by several principles related to CFD and its methodology. The multimedia and dynamic visualization principles are mainly utilized to feed students with content-specific information. Alongside these, we also improve the quality of supporting information with coherence, self-pacing, redundancy, prior knowledge activation, knowledge progression and inductive-expository principle in the modules. Likewise, procedural information is a critical element of the 4C/ID to timely guide users in the learning environment. The fading principle, modality principle, signaling principle, spatial split-attention principle and segmentation principles are spread throughout the modules to help and guide users. In addition, the part-task practice is implemented in the learning practice to get users along with the VR controllers and cognitively challenging aspects of the simulation environment. The recognize-edit-produce principle and component-fluency principle are implemented in the Virtual Garage. Finally, we also use the personalization principle in the Virtual Garage throughout a role-playing scenario. Evidence shows that learning can be more effective with the personalization principle [72]. We only provide an informal conversation style with a human voice narration using a polite communication style to deliver both supporting and procedural information. The narration directly talks to users. We did not implement a visual object to embody the narrator's character. Both audio and written instructions are utilized to deliver supporting and procedural information. All audio instructions are kept compulsory to listen to, even if an accompanying text is available in the same environment.

Table C.1: 4C/ID model and multimedia principles applied in the Virtual Garage concept.

Component	Principles	Examples from the Case#6 in the Virtual Garage
Learning task	Sequential	To enable a learning environment to progressively increase the complexity. For example, first, introduce different types of impellers to mix water. Then add another liquid to investigate the effect of impellers and viscosity on the mixing quality.
	Variability	A non-linear progression across subtasks due to its positive reflection on better test scores. Introduce the power consumption right after the mixing quality to provide a cost-related aspect imperative in decision-making. Then, turn back to mixing quality and examine the effect of baffle plates on the mixing quality.
Supportive information	Multimedia, dynamic visualization, coherence, self-pacing, redundancy, prior knowledge activation, knowledge progression, inductive-expository and personalization	To enable an inclusive experience to deliver complex information, the Virtual Garage inherits a set of principles considering both visual and auditory ways of communication. For example, based on the dynamic visualization principle, users do interact with 3D reactor models and animations to better comprehend components and their functionalities.
Procedural information	Fading, modality, signaling, spatial split-attention, segmentation, personalization	To enable an inclusive experience to guide learners in the educational environment, the Virtual Garage inherits a set of principles considering both visual and auditory ways of communication. For example, based on the signaling principle, users are guided with visual and auditory instructions to proceed with the learning tasks.
Part-task practice	The recognize-edit-produce and component-fluency	In addition, the part-task practice is implemented in the learning practice to get users along with the VR controllers and cognitively challenging aspects of the simulation environment such as checking mesh quality after committing a geometric manipulation.

Available design guidelines on simulator sickness in VR

Interaction and immersion of VR should be cautiously designed to mitigate simulator sickness. In the field of VR, simulator sickness refers to any physical and mental symptoms affecting users' well-being either during or after the VR experience [193]. Literature has recently been bombarded with research on simulator sickness. Several guidelines are made available to lead developers to mitigate simulator sickness in custom VR experiences [193, 176, 177]. The following aspects were taken into account in the Virtual Garage concept and accordingly implemented [193, 176, 177]:

- Hardware: not only software but also hardware can trigger simulator sickness. Commercial ones would alleviate the possibility of simulator sickness if users are guided with regard to design and operating guidelines from manufacturers.
- Display: preferably faster response, better quality, lighter weight, higher refresh rate and resolution.
- Sound: preferably spatialize sound.
- Motion tracking: preferably rapid, accurate and ergonomic.
- Navigation: preferably walking is optimal, optionally teleportation. Avoid flying.
- Ergonomic interactions: 6 degree-of-freedom (DoF) with realistic interface and preferably direct hand interactions.
- User experience: learning interactions via adequate training and time.
- Computer hardware: preferably standalone VR devices.
- Content: simplistic and realistic.
- Visual stimulation: realistic, stable, responsive and low amount of motion.
- Exposure time: less than 10 min or higher than 20 min with simplistic content.

CFD content list and content mapping

Table C.2 illustrates conceptual case studies in order with the complexity of the learning subject, aiming at teaching ultrasound intensified mixing processes in chemical engineering. Cases #5 and #6 are fully digitally produced in the Virtual Garage concept. For the rest of the cases, simulation data are available and already integrated into cross-platform environments to potentially prototype digital applications in the Virtual Garage concept.

The CFD content list was developed considering the prior knowledge of target students. To compile a proper list that can serve both novice and experienced students, we screened the chemical engineering curriculum at KU Leuven,

Table C.2: CFD content list.

CASE	Simulation content from COMSOL, OpenFOAM and Ansys
#1	Flow past solid objects: Karman vortex street
#2	Backward facing step: Sudden expansion
#3	T-junctions (macroscale): Mixing in process industry
#4	T- and V-junctions (milli-scale): Mixing and process intensification
#5	Water treatment basin: reactors with baffle plates
#6	(Continuous) Stirred tank reactor
#7	(Continuous) Oscillatory baffled reactors
#8	Mixing in oscillatory baffled reactors (milli-scale)
#9	Introduction to ultrasound
#10	Ultrasound in Process Intensification
#11	Ultrasound bath processes
#12	Ultrasound horn processes
#13	Ultrasound-assisted oscillatory baffled reactors
#14	Tubular continuous ultrasound-assisted crystallizer
#15	Mixed content to teach fundamentals of CFD (e.g. turbulence modeling)

Belgium. It was revealed that students can struggle with the concept of ultrasound since there are no courses given about the phenomenon, except the very superficial introduction to acoustics in the early years of undergraduate. Similarly, milli- and micro-fluidic applications may also challenge students since the concept is still mostly a matter of research, and only a very limited number of courses cover the basic aspects of such applications. Fig. C.1 shows a content map that comprises content to comprehend process intensification with ultrasound for the unit operations mixing and separation. The branches highlighted with red circles indicate the content that students may lack a fundamental understanding of phenomena.

Learning objectives in the Virtual Garage

In Case#6, students are tasked to design a stirred tank reactor to efficiently mix liquid soap solution using design and operating parameters. Several learning objectives are given to deepen their knowledge of the effect of viscosity, type of impellers, rotational speed and baffle plates. Learning objectives of the learning module Case#6 are aligned with the learning environment. At the end of the Case#6 a student will be able to:

- identify design and operating parameters of a stirred tank reactor;
- predict flow patterns flow patterns for different reactor configurations and working liquids;

- provide advice on how to choose right methodology to design a stirred tank reactor with CFD simulations;
- differentiate design and operating parameters based on viscosity of a working liquid;
- judge efficiency of mixing in a stirred tank reactor;
- configure a stirred tank reactor in order to efficiently high viscous Newtonian liquids such as soap;
- the simulation data was produced by OpenFOAM and COMSOL with incompressible, steady-state, transient and turbulent fluid flow for both 2D and 3D configurations.

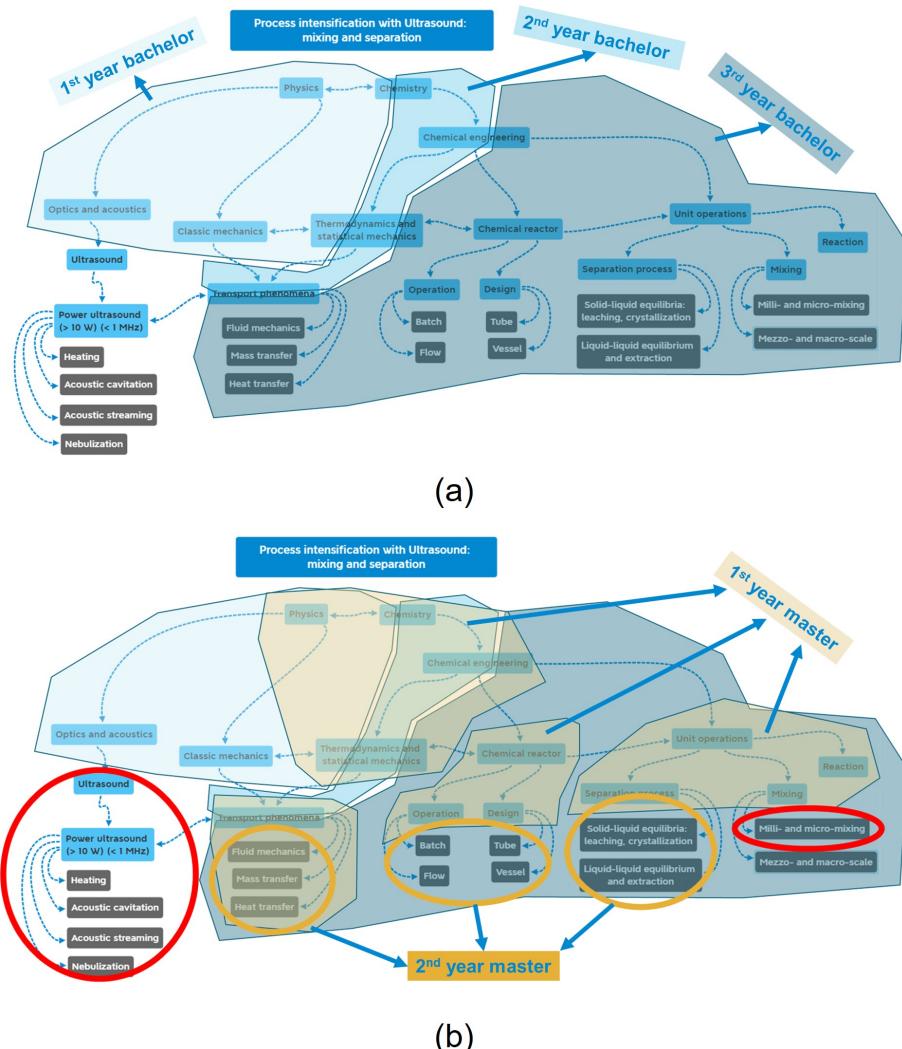


Figure C.1: The content map is created by screening the chemical engineering curriculum at KU Leuven.

Appendix D

Supplementary information for Chapter 6

Free access to the VR application and the walkthrough video

The Virtual Garage with Case#5 is freely downloadable on GitHub: <https://github.com/sersolmaz/The-Virtual-Garage>

A walkthrough video of the Case#5 is available on YouTube: <https://www.youtube.com/watch?v=iJV4jQn7VQY>

The constructs that are not adopted in the conceptual model

There were more constructs than we discussed in our study were appeared in the literature but were not adopted in our conceptual model. First, perceived usefulness and use motivation were employed by researchers in similar contexts. Given the context of our research, we found these constructs superficial to adequately evaluate the behavioral intention. Instead, constructs such as learning value and content value can already give reliable outcomes to interpret behavioral intention from perceived usefulness and use motivation point of view. Secondly, extrinsic value is an emerging factor in behavioral intention since immersive technologies are becoming more invasive in engineering and education. Performance expectancy, content value and learning value do include extrinsic aspects of individuals' behavioral intention to use. Thus, we did not separately measure the extrinsic value in our conceptual model. Furthermore,

Table D.1: UTAUT2 questionnaire with items and constructs adopted from the literature. Items with number sign (#) constitute the immersion (IM) construct.

Construct	Items	References
Performance expectancy	I find the Virtual Garage useful for learning engineering concepts. Using the Virtual Garage to learn engineering concepts increases my engineering knowledge. Using the Virtual Garage helps me learn things more quickly. Using the Virtual Garage increases the quality of my learning experience.	[212]
Effort expectancy	Learning how to use the Virtual Garage is easy for me. My interaction with the Virtual Garage is clear and understandable. I find the Virtual Garage easy to use. It is easy for me to become skillful at using the Virtual Garage.	[212]
Intrinsic value	Using the Virtual Garage is a good idea. Using the Virtual Garage makes learning activities more interesting. Using the Virtual Garage is pleasant. Using the Virtual Garage is fun.	[214]
Learning value	Learning through the Virtual Garage is worth more than the time and effort given to it. The Virtual Garage gives me the opportunity to increase my knowledge and to control my learning experience. At the current context, the Virtual Garage provide a good value in engineering education.	[215, 216]
Self-efficacy	I can use the Virtual Garage, even if there is no one around to guide me. I am confident that I could deal efficiently with most of usability problems in the Virtual Garage. I can remain calm when facing difficulties with the use of the Virtual Garage because I can rely on my coping abilities.	[243]
Content value	The Virtual Garage provides attractive contents. The Virtual Garage provides important and useful contents for my engineering skills. The Virtual Garage makes complex contents and concepts easy to understand.	[219, 244, 221]
Personal innovativeness	If I knew about a new innovation, I would discover new ways to try it out (virtual reality, augmented reality, fluid simulations, etc.). I am keen to try new features available in engineering education provided by university. I would be the first among my friends and peers to try out a new technology. Generally, I like to experiment new features and advancements in information technologies.	[216, 222]
Flow theory	When using the Virtual Garage, I feel absorbed. When using the Virtual Garage, I feel in control. When using the Virtual Garage, I can easily interact with the content and environment. (#) I feel immersed in the virtual reality environment. (#) I feel fully engaged by the virtual reality learning environment.	[92, 245]
Behavioral Intention	I intend to continue using the Virtual Garage to learn again in the near future, if made available for me. I'm open to using the Virtual Garage to improve my knowledge of engineering principles, if made available for me. I plan to continue to use the Virtual Garage to learn engineering principles, if made available for me.	[212]

simulator sickness was considered a significant factor that negatively affects behavioral intention. Due to its vivid effect, we did not extend our model with simulator sickness, which clearly discourages users to adopt VR experiences. Lastly, researchers expanded the UTAUT2 utilizing the satisfaction scale in various contexts. However, in our context, the effect of satisfaction on behavioral intention may not be a sound scale to interpret behavioral intention, because it is still not clear from which point of view the satisfaction should be incorporated into the model. To sum up, there are surely more constructs that can be included to explore various aspects of VR in behavioral intention. Nevertheless, we only considered and discussed the ones given the scope of our study.

Details on Case#5: water treatment basin

Water treatment basins have long been used in industrial-scale processes in order to remove bacteria or other contaminants. Chemicals such as chlorine - valued for both its effectiveness and low cost - are typically used within the water basin to eliminate disease-causing microorganisms in water. The performance of water treatment should be adequate to ensure the disinfection process. CFD simulations are useful tools in the design and analysis of the water treatment performance of a water basin investigating both design and operating parameters. The water treatment basin is an interesting example comprising several aspects of chemical engineering, as well as enabling an introductory case for intensified processes.

In Case#5, students are expected to configure a water treatment basin that satisfies design constraints such as chlorine level and pressure drop. Baffle orientation, size and length are a set of parameters to be optimally chosen by students to comply with constraints. CFD simulations were performed by COMSOL, adopting a case study available on COMSOL's model database. More information about CFD simulations can be found as follows: <https://www.comsol.com/model/water-treatment-basin-14049/>.

Intended learning outcomes are aligned with course content and assessment. They are explicitly defined hard skills and competencies that students are expected to acquire after the learning experience. At the end of the simulations a student will be able to:

- identify design parameters and principles of the water treatment basin;
- identify parameters to predict the performance of water treatment basin;
- predict the effect of design parameters on the performance of the water treatment basin;
- predict the fluid flow patterns for different baffle wall configurations;

- use output data to critically compare design parameters;
- differentiate design parameters by interpreting output data from simulations;
- determine the optimal values for each design parameter;
- formulate a final design for the water treatment basin.

Knowledge test: multiple choice questions

The knowledge test was developed to measure the knowledge gain with eight dedicated questions during the experimental intervention. Students filled the same test before and after the VR experience. Three choices were provided in each question with one correct answer and two credible distractors. The test was validated by peer chemical engineers. Questions in the knowledge tests are shown as follows (*Note that Asterisk (*) implies the correct choice*):

Q1: What parameters are important in the design of a water treatment basin?

- Chlorine residuals, velocity profiles, flow patterns, ambient pressure
- Residence time, chlorine residuals, velocity profiles, flow patterns (*)
- Installation cost, ambient temperature, residence time, flow patterns

Q2: Which of the following best illustrates the significance of the pressure loss in the design of a water treatment basin?

- Pressure loss determines the inlet velocity to reduce operating cost
- Pressure loss determines the size of the pump forcing the flow through the basin(*)
- Pressure loss determines the chlorine residuals and residence time distribution

Q3: Which of the following effects do baffle walls have on the design of water treatment basins?

- Eliminate dead zones, lower pressure loss, better mixing
- Better mixing, higher pressure loss, elimination of dead zones(*)
- Lower pressure loss, better mixing, higher chlorine residuals

Q4: Which of the following parameters are necessary to determine the number of baffle walls in a water treatment basin?

- Pressure loss, chlorine concentration, inlet velocity, flow patterns

- Flow patterns, ambient temperature, chlorine concentration, velocity profiles
- Velocity profiles, pressure loss, flow patterns, chlorine concentration(*)

Q5: Which of the statements below is correct?

- The orientation of the baffle walls does not significantly influence on residence time and pressure loss
- The concentration profile, combined with the flow field, shows regions where the chlorine concentration may increase
- The regions immediately behind the baffle walls have a slightly lower chlorine concentration since these are recirculation zones for the flow(*)

Q6 is available in Fig. D.1.

Q7 is available in Fig. D.2.

Q8 is available in Fig. D.3.

Interest, experience and habit of participants

Respondents came from a diverse background with regard to their interest, experience and habit. Fig. D.4 illustrates the pre-test results completed by students before the VR experience.

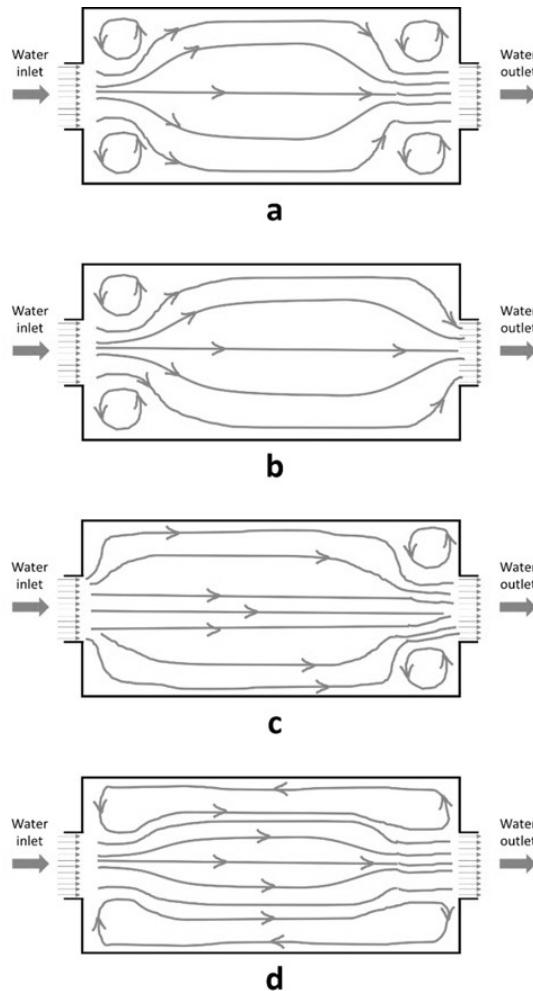


Figure D.1: Q6: Which one of the following correctly illustrates the turbulent fluid flow throughout a water basin? (answer: d).

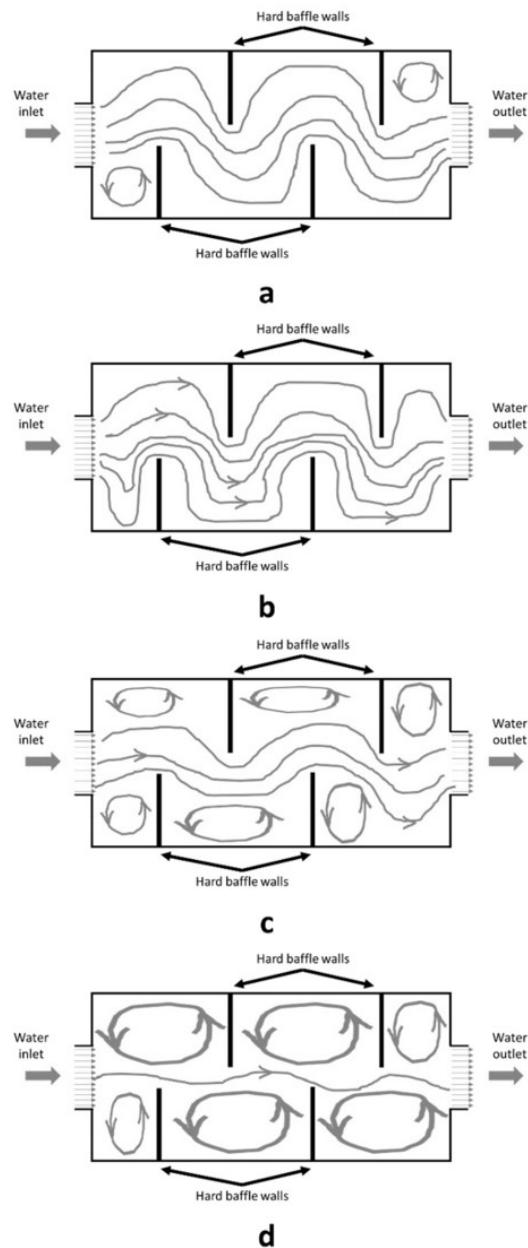


Figure D.2: Q7: Which one of the following correctly illustrates the turbulent fluid flow throughout a water basin? (answer: c).

Table D.2: Bootstrapped Discriminant Validity Hetrotrait-Monotrait Ratio (HTMT) Method.

Constructs	Confidence Intervals		Bias	Corrected	
	Original Sample	Sample Mean		5.0%	95.0%
SE - EE	0.873636	0.870609	-0.00303	0.688268	0.99508
IV - CV	0.819416	0.832651	0.013235	0.600474	0.991098
CV - BI	0.871303	0.870034	-0.00127	0.743181	0.983076
IV - BI	0.848177	0.843867	-0.00431	0.68377	0.965629
PE - LV	0.908571	0.913721	0.00515	0.828865	0.959928
IV - FT	0.820819	0.811197	-0.00962	0.63518	0.952241
LV - BI	0.883408	0.879776	-0.00363	0.770044	0.950255
PE - IV	0.830518	0.837533	0.007015	0.652589	0.945942
PE - CV	0.794179	0.815923	0.021744	0.621182	0.937719
LV - CV	0.806073	0.805938	-0.00014	0.617876	0.934856
PI - IV	0.765012	0.74872	-0.01629	0.533718	0.915574
LV - IV	0.804684	0.799863	-0.00482	0.648465	0.911234
IV - EE	0.715806	0.706975	-0.00883	0.491944	0.894838
PE - BI	0.815067	0.820086	0.005019	0.707965	0.892204
FT - CV	0.738078	0.751006	0.012928	0.567493	0.874604
PI - PE	0.757664	0.75284	-0.00482	0.581326	0.870946
PI - BI	0.735188	0.73068	-0.00451	0.554624	0.86586
PI - CV	0.709287	0.715067	0.00578	0.506829	0.85144
LV - FT	0.655576	0.642283	-0.01329	0.394994	0.826293
PI - LV	0.675822	0.66315	-0.01267	0.467886	0.815751
PI - FT	0.602253	0.592899	-0.00935	0.367186	0.795582
FT - BI	0.66578	0.658851	-0.00693	0.501482	0.789671
FT - EE	0.57156	0.558031	-0.01353	0.317198	0.786116
SE - FT	0.597966	0.593537	-0.00443	0.383143	0.783559
PE - FT	0.548565	0.567855	0.01929	0.308275	0.781213
PI - EE	0.44879	0.449994	0.001203	0.168404	0.76912
SE - IV	0.513996	0.512774	-0.00122	0.26984	0.754429
SE - PI	0.381937	0.394629	0.012692	0.16151	0.656423
EE - BI	0.323873	0.330506	0.006633	0.100312	0.611726
SE - BI	0.312682	0.324938	0.012256	0.098549	0.604009
LV - EE	0.24492	0.285442	0.040522	0.086306	0.567267
PE - EE	0.300168	0.355549	0.055381	0.132033	0.563965
SE - LV	0.236208	0.301996	0.065788	0.084842	0.43605
SE - PE	0.232104	0.294641	0.062537	0.102985	0.423965
SE - CV	0.231883	0.296559	0.064677	0.090903	0.37932
EE - CV	0.2171	0.299273	0.082173	0.090783	0.336439

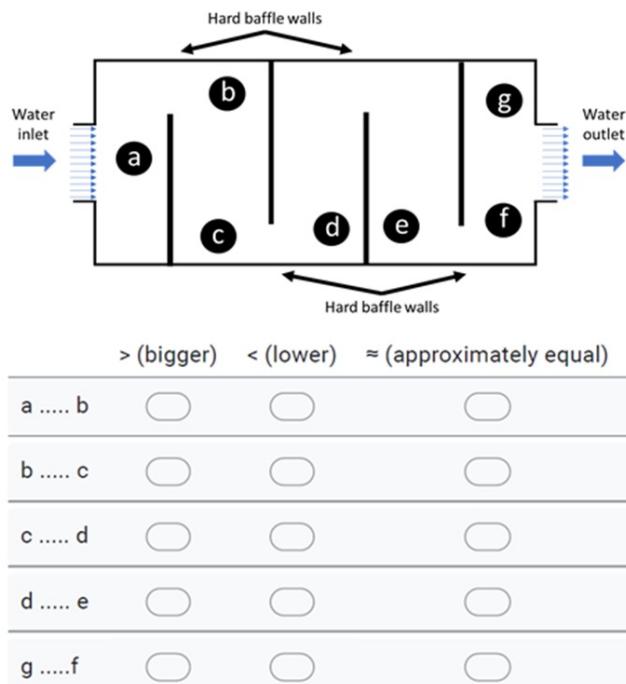


Figure D.3: Q8: Compare the chlorine concentrations of given points in the water basin.



Figure D.4: Interest, experience and habit of participants.

Table D.3: The VIF values. We examined the collinearity to mitigate the effects of bias between constructs. The construct's tolerance (VIF) value was lower than 5 in all items, thus eliminating collinearity.

Collinearity					
Items	VIF	Items	VIF	Items	VIF
	< 5		< 5		< 5
BI1	4.44	IV1	1.811	PI1	1.875
BI2	2.816	IV2	1.749	PI2	1.809
BI3	3.076	IV3	1.515	PI3	2.747
CV1	1.302	IV4	1.467	PI4	2.878
CV2	1.556	LV1	2.643	SE1	3.114
CV3	1.358	LV2	3.436	SE2	3.344
EE1	2.957	LV3	2.482	SE3	1.672
EE2	3.024	PE1	2.416	FT1	1.705
EE3	2.632	PE2	2.886	FT2	1.826
EE4	2.709	PE3	1.758	FT3	1.812
		PE4	2.586	FT4	2.286
				FT5	2.567

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