Enzymes for large-scale processes: an overview of current trends and future perspectives

ENZYMES EMBRACE LARGE-SCALE INDUSTRY: AN OVERVIEW OF CURRENT TRENDS AND FUTURE PERSPECTIVES

Enzymes continue to play a crucial role in various large-scale industrial processes. They are employed for their unique catalytic properties, selectivity, and biocompatibility. This article provides an overview of the current trends and future perspectives in the use of enzymes in large-scale industries. It discusses the advancements in enzyme technology, the challenges faced in their industrial application, and the opportunities for innovation.

1. Introduction

Enzymes are biological catalysts that accelerate chemical reactions, and they are now extensively utilized in large-scale industrial processes. The advancements in enzyme technology have allowed for the optimization of these processes, leading to increased efficiency and reduced costs. However, there are still several challenges to be addressed, such as enzyme stability, process optimization, and cost-effectiveness.

2. Current Trends

2.1. Enzyme Engineering

Enzyme engineering is a rapidly growing field that involves the modification of enzymes to improve their performance in industrial processes. This includes the manipulation of enzyme structures and properties to enhance their stability, activity, and selectivity. Various strategies are employed, such as directed evolution, site-directed mutagenesis, and rational design.

2.2. Enzyme Protection and Stabilization

In large-scale processes, enzymes are often exposed to harsh conditions such as high temperature, pH, and solvent. Therefore, protecting enzymes from these stressors is crucial to maintain their activity and stability. Techniques such as immobilization, encapsulation, and additive screening are used to stabilize enzymes.

3. Future Perspectives

3.1. Personalized Enzymes

The future of enzyme technology involves the development of personalized enzymes, which are tailored to specific applications. This will be achieved through advanced research in enzyme engineering and proteomics.

3.2. Bioreactors

Efficient bioreactors are essential for the large-scale production of enzymes. Innovations in bioreactor design and control will play a significant role in improving enzyme productivity and reducing operational costs.

3.3. Production of Novel Enzymes

The search for novel enzymes with specific properties continues, and this will be facilitated by the advancements in genome editing and directed evolution. These enzymes will find applications in diverse industries, further expanding the use of enzymes in large-scale processes.

4. Conclusion

Enzymes have a significant impact on various large-scale industries, and their use is expected to increase in the future. The challenges in enzyme technology are being addressed, and innovative solutions are being developed to overcome these hurdles. The future of enzyme technology is promising, and it holds great potential for the development of more efficient and sustainable processes.
to be used in production process. In addition, such iterative nature of casting processes is often time consuming and not economically viable in today's competitive world.

The increasing demand of metal casting in mass production has led to the development of virtual casting which refers to the use of computational tools to analyze a casting process. Virtual casting evades the physical trial-and-error approach and makes use of a computational domain to evaluate various casting mold and process designs. This allows methods engineers to proceed with a proof-of-concept approach with all design considerations, process parameters, defect and quality aspects handled prior to a real-time casting process carried out in a foundry. Consequently, the process becomes more efficient by maximizing the casting yield (weight of the casting divided by the weight of the total amount of metal poured) and minimizing the time and cost of production. However, the critical question remained so far is how well virtual casting can replicate the reality and what is its impact on academia, research and industry? While virtual casting aids in improving the overall casting process, it is essential to acquire the detailed knowledge, training, and hands-on experience of the softwares. A number of opportunities can be created at universities and institutes of higher education by establishing labs, periodic training sessions in the industries using casting simulation tools, and providing solutions to metal casting industry through quality centers using high performance computation facilities.

The use of virtual labs in different areas of education has been reported previously by various researchers and educators.2-8 Alexio et al.2 presented the development of an educational virtual laboratory capable of conducting the activities which are normally done in a real laboratory. A web-based system was designed to perform experiments by avatars facilitated with communication and collaboration services. The proposed architecture and basic functionality are discussed. It is suggested that virtual laboratories are preferred in situations where there is risk of students’ life, time consuming experiments, involvement of hazardous substances, cost reduction in constructing a physical lab, and only simulation-based experimentation. It is emphasized that appropriate implementation of a virtual lab is crucial, therefore, it is of utmost importance to (a) decide the educational field to be simulated by virtual lab and (b) conduct a user evaluation about the accuracy of simulations, usability, and friendliness of such an environment. Babateen3 studied the role of virtual laboratory as a model of E-learning and in teaching science. The study provided insights on the concept, components, characteristics, and constraints of virtual learning. The importance of scientific virtual environment is investigated and conclusions are drawn by presenting recommendation and suggestions on virtual lab environment.

Potkonjak et al.4 critically reviewed the state-of-the-art in virtual laboratories in the fields of science, technology and engineering (STE). The study first presented the merits and demerits of virtual systems for education followed by identification of relevant technologies and explanation of recent trends for future developments in technology and application. The use of virtual laboratories in STE is explained by dividing the results into four groups which are (i) general initiatives, (ii) science-physics, (iii) process technologies, and (iv) engineering (nonrobotics and robotics). Owing to high significance of the advanced virtual ambience for establishing a virtual lab, the state-of-the-art in virtual worlds is also explored and substantial restructuring of these virtual worlds is recommended. It is also commented that while virtual lab systems and simulators are currently used only as an initial step in engineering education, it is expected to increase the use of virtual laboratories and reduce the need of real-world laboratories through continued progress in computer graphics, virtual reality, and virtual world systems.
Aljuhani et al.\textsuperscript{5} proposed a virtual science lab (VSL) system to shift the educational system from reality to virtual. System design, user interface design, testing, and results are reported. It is concluded that VSL is a much better approach of conducting the experiments by students instead of just observing them in a physical lab. Moreover, it could be economically feasible together with a better teaching efficiency. However, teaching methods adapted in this scenario should always be modern and flexible to get along with the emerging technologies. Grodotzki et al.\textsuperscript{6} presented the development of a remote and virtual lab of mechanical engineering. The underlying idea of this work was to facilitate linking theory with practice in a virtual environment. A teleoperative testing cell for material characterization is developed to provide students time and location independent access to the laboratory. In addition to this, a teleoperative tube bending cell was also developed for incremental tube bending process. The development of testing cell as a virtual reality lab and a universal virtual experimentation lab are also reported. It is emphasized that with such developments, the future engineering education must include teaching the content of Industry 4.0, for example, automation, big data analysis, and internet-of-things and this should be achieved in a 4.0 manner.

Morales-Mendoza et al.\textsuperscript{7} proposed a hybrid approach of combining virtual and remote laboratories to teach industrial automation courses. The purpose of this work is twofold: (a) reduce high investment and operating costs of equipment and processes in physical laboratories and (b) meet requirement of companies by educating engineers with skills and abilities such as design and implementation of automatic systems for manufacturing processes. In a recent work by Trentsios et al.,\textsuperscript{8} remote labs and virtual reality are combined to benefit from each other thereby enhancing the educational value. The creation of a virtual environment is proposed by establishing two different approaches: (i) 360° imaging to represent the physical lab and (ii) a virtual three-dimensional (3D) model of existing physical lab. The constraints with remote labs such as single user interaction at a time are identified and suggested conversion of remote lab into a virtual lab which not only simulate the behavior of actual lab but also can be accessed by multiple users simultaneously.

This article presents an initiative on \textit{Virtual Metal Casting Lab} taken by King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia. In line with the literature presented above, the main objective of this work is to communicate the importance of virtual casting in education and research, and to provide a framework for establishing and developing a virtual casting lab to expand research in manufacturing. Casting simulation softwares are introduced briefly. Next, the establishment of virtual casting lab at KFUPM are discussed which summarizes acquiring licenses of a casting simulation software and its training, collaboration with the local industries, learning and capacity building at KFUPM in several stages, and so forth. A detailed discussion on the utilization of casting simulation software by students, instructors, and researchers is included which advocates the expertise developed at KFUPM by working on enhancing the quality and integrity of metal cast products of Saudi foundries. Finally, the future plans related to expansion of virtual metal casting lab leading to a \textit{Virtual Casting Quality Center} for its continued support to academia, research, and industry at a larger scale are presented.

2  |  VIRTUAL CASTING SOFTWARES

The modeling and simulation of a casting process in virtual domain is tricky due to a host of parameters involved such as pouring temperature, cast material properties, fluid velocity, pressure, geometry of the mold, gating, runner system, and so forth. Taking into account all important factors which can directly and indirectly influence the process is a key to develop a casting simulation software. A range of softwares that have been emerged over time are a result of understanding the physical phenomena during a casting process. The relevant mathematical models are either developed or modified and then implemented into computer programs to develop a software.\textsuperscript{9} Some of the most commonly used casting simulation softwares which are currently available to researchers and foundrymen are listed in Table 1.

Virtual casting generally comprises of five stages as shown in Figure 2. These five stages are data gathering, methods design, numerical simulation, methods optimization, and project conclusions.\textsuperscript{10} Data gathering refers to all information needed related to CAD model of casting, cast metal properties, mold properties, process parameters, and so forth. Method design and modeling primarily focuses on how to convert the as cast part model into a 3D mold which contains cavities, gating system, runners, risers, cores, and feed-aids. Next, the numerical simulation is done after generating the optimum mesh and defining boundary conditions. Visualization of results is done by a postprocessing module in each simulation software. With the simulation results, it is often possible to identify defects such as hotspots, microporosity, shrinkage, cold shuts, and others. Therefore, a step forward in simulation is methods optimization which includes modifications in gating and riser designs, process parameters and material properties, and even in part model to minimize the defects.
The final stage which is termed as project closure includes complete documentation of results, generating methods and analysis reports, capturing images and animations for demonstration at the later stage.

Virtual casting begins with modeling the physical phenomena through mathematical equations. In a mathematical perspective, models are expressed as governing equations and boundary conditions. Owing to the nonlinearity of models in terms of both geometry and material properties, numerical methods have to be used to avoid nonlinearity and thus formulate simultaneous and algebraic equations. The set of developed equations is then used to explain casting process in the form of action-behavior-property relationship. For a metal casting process, the action is supplying molten material to the mold, the behavior is the flow of molten metal within the mold, and the behavior is further decided by properties of the molten metal. From modeling point of view, three important phenomena in any casting process simulation are mold filling, solidification and cooling, and stress and strain profile of the cast parts. The numerical methods for solving the equations are finite difference method (FDM), finite volume method, finite element method (FEM), vector element method, cellular automation method, and so forth. Sometimes a combination of two or more techniques may also be employed, the examples of which are cellular automation finite element method proposed by Rappaz and Rettenmayr, and a hybrid method for casting process simulation by combining FDM and FEM. The final simulation results, however, are representative of casting process and properties, qualities and defects of cast products irrespective of the type of solutions discussed above.

Virtual casting results in three major aspects of a casting process: filling, solidification, and stress analysis. Each of these three simulation types reveal sources and causes of casting defects and thus provide an opportunity to rectify any errors. Mathematical modeling and simulation of conservation of mass, momentum, and energy in a filling process provides information about velocity of molten material within the mold cavity, the direction of flow, temperature, and pressure at various instances within the mold. Physical and thermal characteristics of the filling process are derived from these results, some of which are flow front progression, turbulence in flow, filling evenness, air and gas entrapment, temperature profile, filling sequence, velocity profile of molten metal, odd behaviors such as splashing, misruns, cold shuts, and so forth during filling. Solidification in casting process is generally complex, where physical, thermal, and metallurgical phenomena take place simultaneously. Solidification simulation provides information about how these phenomena are occurring in process conditions together with the defects that might arise during solidification phase. Some key findings of a solidification simulation include cast area that solidifies last, solidification sequence, validation of cooling design, validation of runner design, defects due to shrinkage and microporosity, appropriate riser geometry, size and location

### TABLE 1  Casting simulation softwares

| Software program         | Company and location                      |
|--------------------------|-------------------------------------------|
| AutoCAST                 | Advances Reasoning Technologies P. Ltd., Mumbai |
| CAP/WRAFTS               | EKK, Inc., Willed Lake, MI, USA           |
| CastCAE                  | CT-Castech Inc. Oy, Espoo, Finland        |
| Castflow, Castharm       | Walkington Engineering, Inc., Australia   |
| JSCast                   | Komatsu Soft Ltd., Osaka, Japan           |
| MAGMASoft                | MAGMA GmbH, Aachen, Germany              |
| MAVIS                    | Alphacast software, Swansea, UK           |
| Nova-Solid/Flow          | Novacast AB, Ronneby, Sweden              |
| PAM-CAST/ProCAST         | ESI Group, Paris, France                  |
| RAPID/CAST               | Concurrent Technologies Corp., Johnstown, PA, USA |
| SIMTEC                   | RWP GmbH, Roetgen, Germany               |
| SOLIDCast                | Finite Solutions, Inc., Illinois, USA     |

### FIGURE 2  Simulation and optimization protocol in virtual casting
within the mold. The stress and strain simulation demonstrates the state of cast parts after ejecting from the mold. The results of these simulations may include identification of dimensional inaccuracies, residual stress generation and distribution in cast part, defects arise due to stress and strain, temperature profile in ejected cast part, design improvements in casting design such as modifications in riser design to reduce stresses and so forth.

3 | ESTABLISHMENT OF VIRTUAL CASTING LAB AT KFUPM

The concept of building a virtual metal casting lab dates back to 2007 when MAGMASoft, a high end casting simulation software, was acquired as part of extensive bundled purchase of Finite Difference Method (FDM) machine, MK Technology, vacuum casting machine, FaroArm, and several other softwares. The software was acquired with an aim to utilize it only for educational/academic/research and not for any commercial purposes. MAGMASoft was installed on three Linux-based personal computers by MAGMA representatives together with a short training program on introduction and how to use MAGMASoft. Since then, KFUPM–MAGMA collaboration continued to grow as evident by several events mentioned in the timeline shown in Figure 3. This relationship was mutually beneficial as KFUPM utilized MAGMA support in producing research products in the form of students’ projects, theses and dissertations, and research publications, whereas, MAGMA got its outreach to industry through one of the top institutes in the region.

The expertise developed at virtual casting lab results from continuous training and support from MAGMA. In this regard, training sessions and a seminar have been arranged at KFUPM campus. A technical seminar/workshop on “Metal Casting Simulations Quality and Productivity Improvement by MAGMASoft” was arranged in February 2013 at KFUPM campus. Both MAGMA Germany and MAGMA Turkey participated in the seminar along with the local participants from Saudi ARAMCO, SMI Riyadh, and other local industries. The seminar started with a live demonstration on “How to work with MAGMASoft?” followed by various industrial examples covering utilization of MAGMASoft for steel applications, prediction and minimization of stresses and cracks in steel castings, advantages of casting simulations in an iron foundry and so forth. The perspective of local industries was also presented, discussed and conclusions drawn. In 2015, a 2-days training session by MAGMA representatives from Turkey and Egypt was held at KFUPM with MAGMASoft (Version 5.2) installed on Microsoft Windows. The users of virtual casting lab were trained for filling and solidification simulations in MAGMASoft. Many additional features of the software were introduced during this training session some of which are creation of control points to monitor simulations instantaneously, controlling the mesh, pouring constraints, start simulation settings, queued simulations, and so forth.

Following up this training, another 2-days training session was organized in 2016, during which a MAGMA representative from Egypt installed the latest version of MAGMASoft (Version 5.3) on the PCs in virtual casting lab at KFUPM. This upgrade of MAGMASoft brought systematic and autonomous optimization to virtual casting lab which refers to an automatic trial and error approach in a virtual domain based on user-defined goals/objectives such as minimum porosity, maximum yield, minimum oxides, improved mold/die life, and so forth. The software simulates all possible combinations and makes decision to improve materials properties and/or process parameters. This approach saves a lot of time due to limited human interaction in contrast to conventional simulations where each simulation has to be set by user based on improved design and process conditions. In general, autonomous optimization simulations result in identifying the best design for gating and riser (locations and dimensions) system, placement of chills, runner dimensions, and so forth and process parameters such as pouring temperature, pouring rate, and mold/die temperatures can also be optimized. Some of the outcomes of both the training sessions are presented in the section on utilization of MAGMASoft at KFUPM virtual casting lab.

It is obvious to verify the outcomes of a casting simulation through physical experimentation. Besides the available on-campus facilities to validate the conceptual designs and simulation results obtained in virtual casting lab, the university started to collaborate with the Axles, Foundries & Spare Parts Factory—MASABIK, which is one of the largest and most advanced foundries in Saudi Arabia. Gray and ductile iron, and steel castings can be produced at MASABIK with the casting layout designed by students and researchers at KFUPM. The capabilities of virtual casting lab such as improved casting designs with minimum defects, minimized production times, and reduced product costs persuaded MASABIK
to include virtual casting as an integral component in their production cycle. For this purpose, MASABIK purchased commercial license of MAGMASoft to be used in their foundry projects which suggests the expansion of virtual casting in Saudi Arabia beyond academia and research. The linkage between virtual casting lab and industry was not just limited to MASABIK, rather, KFUPM also approached SAUDI ARAMCO (the National Petroleum and Natural Gas Company being a major end user of cast parts such as valves and so forth) with a vision to build a Casting Quality Center at KFUPM. The understanding of some initial support from the collaborating industries (MASABIK and SAUDI ARAMCO) invigorated the users of virtual casting lab to initiate proposals for research support and funding from National Science, Technology and Innovation Plan (NSTIP), Saudi Arabia. Out of the two proposed projects, one is completed and the other is on-going, the details of which are presented in the forthcoming sections.

4 | UTILIZATION OF MAGMASOFT AT KFUPM VIRTUAL CASTING LAB

As discussed earlier, the utilization of MAGMASoft at KFUPM’s virtual casting lab is genuinely for academic, educational, and research purposes. If categorized broadly, MAGMASoft is utilized by students, instructors and researchers in (a) Junior and senior level courses in undergraduate teaching (b) Senior design projects in undergraduate program, (c) Theses and dissertations in graduate program, and (d) Research projects funded by NSTIP. Following subsections explains how virtual casting lab in general, and MAGMASoft in particular, provides academic and research support to achieve the goals set in one of the domains from (a) to (d).

4.1 | Junior and senior level courses in undergraduate teaching

A conventional method to teach undergraduate manufacturing courses with an element on metal casting is to introduce students with the fundamentals of casting, casting processes, mathematical aspects of casting design and solidification time and so forth, and a visit to a physical casting lab for a simple demonstration. However, modern teaching methods of teaching manufacturing courses brings about a need of integrating class room instruction, simulations, and physical lab experiment. Erdem and Sirinterlikci15 suggested this integration using a three-tiered approach which incorporates various elements to reinforce the learning process while accomplishing its objectives. The first tier focuses on classroom lectures where the above mentioned various aspects of casting processes are introduced including underlying laws of physics. Second tier is related to computer simulation to actively engage students in the learning process. Finally, the third tier constitutes the hands-on laboratory experience.

Most of the junior and senior level courses at KFUPM comprise of lectures and laboratory sessions. Prior to the establishment of virtual casting lab, metal casting related concepts were taught in classroom followed by metal casting experiments in a physical metal casting laboratory. It can be fairly said that second tier of the integration proposed by Erdem and Sirinterlikci15 was missing in delivering the course. The development of virtual casting lab added a new component on simulation to laboratory work for manufacturing courses such as Manufacturing Processes, Manufacturing and Design, Casting and Welding Engineering, and so forth. During lab sessions students are introduced with the software MAGMASoft and experimental facilities. Besides the routine experiments on sand casting with both permanent and expendable patterns, the students are also encouraged to use the available computational facilities in the lab to work on their short projects or even term projects during the course of the semester.

4.2 | Senior design projects in undergraduate programs

Senior design project is done in partial fulfillment of the undergraduate degree program at KFUPM. Senior students work on their projects by spending 4–6 h weekly in the lab throughout the semester. The existing facilities in virtual casting lab are also used to work on metal casting related projects. Some of the completed projects are as follows.

(a) Lost foam casting process
(b) Design of optimized molds for making quality metal casting products
(c) Pattern and mold design for nonferrous metal castings
(d) Sand casting design for ferrous materials
(e) Design issues in using rapid prototyping technologies in metal casting processes
Senior design project provides an opportunity for students to practically implement their theoretical knowledge already acquired in junior and senior level courses. In particular, a typical metal casting project using virtual casting technology enable students to understand the physical phenomena during casting process in great detail, design the casting layout using CAD tools (Solidworks), decide upon casting process parameters, and computationally analyze the process through casting simulation softwares. One such example is presented in Figure 4 where a simple part is selected for CAD modeling, casting layout design and simulation using MAGMASoft.

### 4.3 Theses and dissertations in graduate program

#### 4.3.1 Improving quality and productivity of casting process by using advanced simulation and rapid prototyping technology

This study was aimed to show the benefits of simulation in casting process to minimize the production time and to achieve a high quality casting. The main objectives defined were:

(a) Development of mold design strategy for semicomplex geometry by adapting the industrial best practices in sand casting process

(b) Analysis of flow behavior and effect process variables such as filling time, filling velocity, filling pressure, and solidification rate on casting quality indicators such as air entrapment, hot spots, porosity, or shrinkage by simulations.

(c) Validation of simulated mold design, reduction in mold development time, improved product quality through experimentation

(d) Metallurgical study of the casting at selected locations to study the effect of solidification rate on microstructure development.

A flow diagram of the research is presented in Figure 5. The selected part for this work was a pump impeller as shown in Figure 6. This part was selected as it is widely used in industry and it is mostly cast by sand casting due to its moderately complex geometry. In addition, it contains both thick and thin sections to analyze the effect of process variables on casting quality. Initial mold design, that is, Design 1 as shown in Figure 7(A) was based on methodology and
formulae available in Reference 16, which was modified in subsequent stages as shown in Figure 7(B,C) using virtual casting. The casting in mold was oriented in such a way that the thin area was in the cope. Based on simulation results for Design 1, the cast body in Design 2 was inverted so that the thin area lied within the drag. Also the location of feeder was changed to the top of porosity concentration area as shown in Figure 7(B). Design 3 was a modified version of Design 2 with an aim to increase casting yield by reducing the volume of gating design. This modification was based on JICA standards.17

Simulation results for all three mold designs are presented in Figure 8. It can be observed that the Design 1 resulted with significant air entrapment and porosity which was reduced in Design 2 and further optimized in Design 3. The hotspot in Design 1 was not eliminated in Design 2, however, the hotspot was completely shifted to riser in Design 3, thereby, eliminating this defect. It was reported that Design 3 also provided a better yield together with complete removal of porosity and hotspot from the cast part.
Considering Design 3 as optimal mold design, it was selected for experimental validation though actual sand casting process. For this purpose, a pattern of the impeller was created using FDM technique. The process of making pattern using FDM and the resulting pattern are shown in Figure 9(A,B), respectively. Next, a sand mold is prepared using the pattern along with the same gating system and riser as obtained in optimal mold design. The mold and the final cast product are presented in Figure 10(A,B), respectively. The final casting obtained after minor machining revealed no defects as predicted by the casting simulations which reflected the effectiveness of virtual casting in obtaining a near optimal mold design using less resources and time.
4.3.2 Optimization of quality and productivity of zinc alloy castings by using advanced simulation techniques

This research was focused on casting nonferrous metals by comparing gravity casting and spin casting processes. Certainly, die casting is preferred for casting a large production volume (10,000–100,000). However, for medium (500–10,000) and small (1–500) production volumes, spin casting and gravity casting processes can be considered, respectively. Since, spin casting process cannot be simulated using MAGMA, therefore, the simulations in this project were limited to gravity casting process. For gravity casting process, three mold materials were used, that is, sand, plaster, and ceramic. The mold was designed, simulated and optimized using MAGMASoft simulations and the near optimal mold design was used for casting zinc alloy.

The initial mold for casting specimens and design modifications are shown in Figure 11, and the corresponding simulation results for each mold design are presented in Figure 12. The simulation results were then validated through experiments. For sand casting, a two-piece split mold was made by green sand as shown in Figure 13(A). Similarly, for plaster mold casting, the mold was prepared using gypsum powder as shown in Figure 13(B). The ceramic mold, however, was 3D printed using Z printers as shown in Figure 13(C) to analyze the feasibility of pattern-less, direct metal casting. A complete experimental setup for spin casting process was also arranged where silicon mold was prepared using a vulcanizing press as shown in Figure 14. The mold after vulcanizing was hard and precise in dimensions of the cast parts. Parametric study on process parameters for spin casting, and quality comparison between gravity casting and spin casting processes were also done as part of this study.

**FIGURE 11** Mold design for casting specimens (A) Design 1, (B) Design 2, and (C) Design 3

**FIGURE 12** Simulated temperature profile within the mold for (A) Design 1, (B) Design 2, and (C) Design 3
4.3.3 Development of a simulation-based methodology for mold design optimization and reliability assessment of cast parts

The main objective of this work is to develop a methodology for cradle to grave analysis of castings in a virtual domain by utilizing advanced metal casting and FEM-based simulation tools as well as validation of methodology using some simple casting geometries. These tools are used in an integrated manner to analyze from mold design to failure of some typical high valued parts. A flow diagram of this research is presented in Figure 15.

The simple geometries selected for methodology development and validation are tensile test and fatigue test specimens as shown in Figure 16. For casting test specimens of both types, multicavity molds with sprue-runner configuration are designed and simulated using MAGMASoft in virtual casting lab. For brevity, only final mold designs are presented in Figure 17. Figure 18 presents the simulation results of the final mold design for porosity and hotspot.
**FIGURE 16** (A) Round specimen for fatigue loading (B) rectangular specimen for tensile loading

**FIGURE 17** Multicavity mold design for (A) tensile and (B) fatigue specimens

**FIGURE 18** Simulated porosity and hotspot in final mold design using MAGMASoft\textsuperscript{18,19}
Followed by simulations, the wooden patterns are produced to create sand molds as shown in Figure 19. Patterns are made and casting of specimens is done at collaborating industry MASABIK. The mold halves for both tensile and fatigue specimens are presented in Figure 20 and the cast specimens prior to final machining are shown in Figure 21. The specimens presented in Figure 21 are machined to final dimensions and are tested under tensile and cyclic loading. The same tests are simulated by integrating the MAGMASoft results in a finite element software (ABAQUS or ANSYS) in the virtual casting lab. After the methodology is validated, the cradle to grave analysis of selected moderately complex parts is done only in virtual domain to analyze their mechanical performance.

4.4 | Research projects funded by NSTIP

The facilities at current virtual casting lab have been used to work on externally funded projects from NSTIP. One research project has been completed in 2013 whereas another project is completed recently. The details of both projects are provided in the following subsections.

4.4.1 | Rapid castings of nonferrous and ferrous parts by deploying innovative pattern and mold making technologies using green sand, plaster/ceramics, and polymers

This project was a mix of development (50%) and research (50%) activities where the research component was heavily dependent upon the various lab facilities developed during the project. The project proposed a number of new foundry strategies which permits the rapid and cost effective production of customized single, small, and medium volume complex shaped cast parts. The research was focused on casting developments incorporating pattern making by Rapid Prototyping
and Spin Casting in addition to direct mold production by Z-Cast technology. Moreover, the quality of the products made using these technologies, and their impact on sand casting, shell casting, and ceramic mold casting processes was also assessed. The quality characteristics and limitations of molds made by this route were analyzed. It was determined that these RP technologies for producing patterns, and virtual simulation tools, can effectively be integrated in any casting process with several beneficial results some of which are

- Ability to make complex patterns, and cores (directly printing by Z printing).
- Ability to conduct virtual casting process simulation using MAGMASOFT, in accordance with parameters of actual foundry practice.
- Ability to visualize filling patterns, velocity fields, pressure gradients, solidification temperatures, temperature gradients, hot spots, hot tears, porosity, and microporosity at any location in the casting. These results combined with metallurgical knowledge help to realize iteratively an optimized and streamlined mold, which can be the starting point of actual casting from virtual to physical domain.

A state-of-the-art RP and 3D printing facility was developed to provide modern materials processing technology a combination of RP and various metal casting routes. Some of the key development activities during this project are installation of 3D printers for direct printing of molds, laminated object modeling machine for producing solid plastic models/casting patterns, 3D subtractive rapid prototyping machinery for creating high resolution patterns of small size from chemical wood, hard machine-able wax or acrylic/plexiglass, Casting software MAGMASOFT, Complete Spin Casting facility with consumables by TEKCAST and so forth.

The use of MAGMASoft during this project confirmed that the mold development time can be reduced by optimizing the mold using advanced simulation tools.\(^\text{20}\) By optimization, it refers to a comparison among various feasible options of gating systems out of which the one with least problems and no quality defects is selected for actual casting. Such optimization leads to less mold development efforts in physical production of the mold. Sequential simulations enables to arrive at a mold which also gives the best yield, and can help to further reduce the recycle cost of material cut from the casting in preprocessing. A case study was done for a spring flap (a thick steel plate with multiple thickness). The study began with developing a solid CAD model of the spring flap along with the gating system design. Based on the defects observed in simulation results, the mold design was optimized in three stages. Results at each stage are verified through actual casting of the part. Figure 22 represents the part model and prediction of defects (porosity) from MAGMASoft at each stage of design improvement.

### 4.4.2 Enhancing quality and integrity of metal cast products of Saudi foundries through advanced simulation tools

This project is focused on improving the quality of cast products used in Saudi industries such as ARAMCO, SABIC, and so forth. These cast parts are mostly made up of ductile iron and different types of steel, which are often subjected to dynamic loading conditions in service. Local foundries cast these parts with a certain level of expertise and usually they are found to be defect-free. However, experience suggests that some critical defects may remain undetected and as a consequence, they show up when product fails during its service life. This project is aimed to provide corrective actions to minimize such failures by developing stringent acceptance criteria for such critical high value parts.

Part of this project work is already explained in Section 4.3.3. Besides the methodology development and validation for cradle to grave analysis of cast parts in virtual domain, the outcomes/deliverable of this project are as follows.

(a) Guidelines for acceptance criteria of cast parts by end users (such as ARAMCO or other similar entities).
(b) Development of research products and intellectual property.
(c) Development of educational and qualification products.
(d) Extension of virtual metal casting lab at KFUPM
(e) Developing Pathway to a physical metal casting lab at KFUPM
5 | EVALUATION OF VIRTUAL CASTING LAB

The virtual casting lab proved to have a positive impact on researchers, faculty, and students by increasing knowledge and expertise in the area. Following are the results obtained by this lab.

(i) Addition of virtual casting lab in courses on manufacturing and casting and welding engineering is considered as a stepping stone towards learning through a virtual environment. It was not only appreciated by students rather the students started to use the lab in miniprojects for courses and to conceptualize their senior design projects with the faculty involved in this lab development. In an informal discussion with the students, their main motivation is to learn new skills along with the formal engineering education which are demanded by organizations during the employment process.

(ii) The graduate students and researchers considered this lab as an excellent research platform. The whole team involved in this lab development was trained with a high-end casting simulation software. In their opinion, more people should be trained to make the most of this lab and an extension of lab to casting quality center will definitely bring a lot of funding opportunities from the participating industries.

(iii) The research funded projects completed by using this lab generated significant scientific contribution through conference and journal publications. It is expected to develop more intellectual property by utilizing the facilities available in lab.

(iv) Some challenges are identified such as immediate validation of castings simulations is not currently possible within the university. Students and researchers have to approach local foundries for such experiments. However, as mentioned in Section 4.4.2, the team is also developing a pathway to a physical metal casting lab within university.

6 | EXTENSION OF VIRTUAL CASTING LAB LEADING TO CASTING QUALITY CENTER

At present, Virtual Casting Lab exists within the Rapid Prototyping and Reverse Engineering lab at KFUPM with three MAGMASoft licenses installed on PCs. However, an extension in the lab is within the scope of NSTIP project discussed in
Section 4.4.2. A layout of the proposed lab is presented in Figure 23. In order to fully utilize its capabilities, the enhanced virtual metal casting lab will be tentatively equipped with the following.

(a) Six high performance desktop systems  
(b) High performance laptops  
(c) HP color printer and cartridges  
(d) Three new licenses of MAGMASOFT complete package and upgrade of three old licenses of MAGMASOFT.  
(e) Team viewer cooperative version.

7 | CONCLUSIONS AND FUTURE WORK

The establishment and accomplishments of a virtual lab in engineering education are presented in this article. In particular, the role of a virtual lab in improving the quality of metal castings is discussed. Following are the conclusions, scientific contribution, and future recommendations resulting from this work.

Engineering education is continuously benefiting from virtual learning methodologies. Owing to high cost and time associated with physical trial and error approach in metal castings, it is extremely important to visualize the process sequence and set the process parameters by simulating the casting run in a virtual lab environment. Nevertheless, the need of physical lab coexists to manufacture the part for its end use.

Learning virtual casting at undergraduate and graduate levels is necessary for engineers who wish to pursue a career in foundries. This helps in a better understanding and handling of casting simulation packages for replicating the real process in a virtual domain. With this aim, virtual casting facilities are developed at KFUPM which showed significant progress over the past few years as reported in case studies and projects in this article. It should be noted that this study is limited to qualitative analysis of learning outcomes of virtual casting lab. Although, the courses in which the lab is utilized are already examined for course learning outcomes, so far, no direct/indirect measurement of learning outcomes is done only for the lab. At this stage, the successful completion of funded research projects and scholarly outcomes such as journal articles and conference articles generated by the lab are presented as a qualitative mean to understand the effectiveness of this lab as an educational tool. It is planned to quantify the learning outcomes directly and indirectly. The direct measurement can be performed by including a course learning outcome on the use of lab in the course specification of all courses where this lab is utilized. Indirect measurements, on the other hand, can be performed through course learning outcome surveys where all lab users must participate such as undergraduate and graduate students, researchers, instructors, and so forth.

Since, introducing virtual reality in engineering courses is challenging due to an extensive use of physical labs for hands on experience, the work presented here is a source of encouragement to other institutes and universities to develop virtual labs in different areas of engineering. In addition, it provides a framework on how such developments can be
made using different building blocks so that a course with no virtual element can be modified and equipped with a fully functional virtual lab which can be integrated to lectures, experiments, design projects, and so forth.

The activities reported in this article have also led to the idea of developing a casting quality center in collaboration with the end users (ARAMCO/SABIC and so forth), local casting companies (MASABIK, SMI, and Saudi Cast), KFUPM (Rapid prototyping lab/ME Department) and casting simulation software company (MAGMA). A quality center of this nature can act as a bridge between universities and industries thereby solving problems of expertise and funds between these two entities.

In terms of future work, casting quality center needs to be planned further for automation and remote access by its expected users. Once, the quality center is developed and fully functional in obtaining robust casting designs using virtual techniques, it can be extended for a safe metal casting unit using robots within the lab where castings can be produced on a lab scale for demonstration purpose.

Finally, the article provides a new perspective to metal casting with respect to industry 4.0 revolution where the traditional metal casting practices are combined with latest smart technologies. The need of being more reactive to customer needs together with maintaining productivity, integrity and efficiency seems possible only through a mix of physical, virtual, and digital metal casting.

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