Technical University of Košice

Faculty of Mining, Ecology, Process Control and Geotechnologies

Design and implementation of modern methods for modeling and control of technological objects and processes

2020

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Study Programme:	Process Control
Field of study:	Cybernetics
Department:	Institute of Control and Informatization of Production Processes (ÚRIVP)
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Košice 2020

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Technická univerzita v Košiciach

Fakulta baníctva, ekológie, riadenia a geotechnológií

Návrh a implementácia moderných metód modelovania a riadenia technologických objektov a procesov

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Návrh a implementácia moderných metód modelovania a riadenia technologických objektov a procesov

Študijný program:	Riadenie procesov
Študijný odbor:	Kybernetika
Školiace pracovisko:	Ústav riadenia a informatizácie výrobných procesov (ÚRIVP)
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Košice 2020 **Ing. Michal Takáč**

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1 Introduction

The objective of process control is to keep key process-operating parameters within narrow bounds of the reference value or setpoint. Controllers are used to automate a human function in an effort to control a variable. A basic controller can keep an individual loop on an even point, so long as there is not too much disruption. Complex processes like ones in metallurgy might employ dozens or even hundreds of such controllers, but keeping an eye on the big picture was, until not so long ago, a human process.

Although a device was used to automate a human function in an effort to control a variable, there was no sense of what the process was doing overall. A basic controller could keep an individual loop on an even keel, more or less, so long as there was not too much disruption. Complex processes might employ dozens or even hundreds of such controllers, each with its performance displayed on a panel board, but keeping an eye on the big picture was still a human process.

When distributed control system (DCS) platforms were introduced in the 1970s, they simplified the mechanics of the panel board, but did not do much to improve its capabilities. Big-picture analysis was still largely a human responsibility. Sure, getting beyond the technical constraints of pneumatic field devices with their troublesome compressed air tubing made it easier to install more instruments and actuators, but the basic control concepts did not really change. Any movement to advanced process control (APC) and other forms of control optimization were still in their infancy. Process automation capable of supporting APC had to encompass many technologies and techniques. It was characterized by incorporating many more input data points into algorithms and orchestrating more complex sequences.

The transition to process automation and advanced process control (APC) was empowered by being able to create an all-encompassing platform capable of coordinating more than single loops or small cascade groups. One major advantage of newer platforms is the ability to optimize a process to suit the owner's specific economic goals based on any number of desired outcomes. The process automation system can operate the plant to minimize energy consumption, maximize output, and deliver specific product quality attributes.

Implementing such systems is challenging. During the initial design phase of a control system upgrade or a new installation, it is far too easy to focus just on process fundamentals, and never get beyond considering desired steady-state conditions. Automation system upgrades and new installations can therefore miss opportunities to engage with process and automation technology experts capable of uncovering better ways of doing things. Many capabilities of modern process automation systems are still underutilized in most process plants. Far fewer companies use APC as effectively as they could, even though basic APC technologies have been around for decades.

Peter Drucker, a well-known management thinker, who has been quoted multiple times over the years by various people, has famously said: “If you can’t measure it, you can’t manage it. If you can’t manage it, you can’t improve it.” His words are now resonating more than ever with the push towards Industry 4.0. New trends like smart sensors, parallel computing for fluid dynamics simulations and virtual reality are getting traction and they found useful applications in metallurgy field, especially in production processes. Roadmap for implementing Industry 4.0 solutions into practice is being pushed around the world and we can feel it happening intensely in Europe region as well. Integrating them into already established plants is not coming without big considerations and analyses of potential economic benefits. Employing smart sensors that can gather and generate multiple-times more data means we must also employ more efficient algorithms for processing these large amounts of data. Data sets on the steelmaking process were available before, however the innovations of the fourth industrial revolution are opening new conceivable outcomes that permit steel makers to gather more information in various manners from myriad of smart sensors and smart systems that communicate over a local network. The term ”Big Data” refers to this phenomenon of increasing complexity that it’s difficult or impossible to process using traditional methods and also volume and velocity of data acquisition we now see regularly with upcoming fourth industrial revolution. Big Data means the analysis of large amounts of data coming from different sources with high speed and with the aim to create economic benefit.

The goal of this disseration is to encompass applications of selected procedures that fall under the umbrella term Industry 4.0 in metallurgy field, specifically in basic oxygen steelmaking process (BOP), by connecting latest research in process control, mathematical modeling, numerical simulation, computational fluid dynamics, visualization and virtual reality. With combined expertise from my work in software engineering, 3D modeling and virtual reality visualizations with research work done by colleagues at Institute of Control and Informatization of Production Processes, novel immersive virtual reality environment for studying basic oxygen steelmaking processes will be designed and implemented. Objectives of the dissertation will be discussed in section 3. I find it useful to focus specifically on this area as I have access to good research opportunities in my region (U.S.Steel in Košice, Vöestalpine in Linz), and last, but not least, BOP is one of two major commercial processes for making steel (other being electric arc furnace).

2 State of Art

In this section we deal with the current state of the art of process control, simulation and visualization in general and also concentrating on elementary processes in the oxygen converter used in steelmaking. There have been tremendous improvements in iron and steelmaking processes in the past twenty years. Productivity and coke rates in the blast furnace and the ability to refine steel to demanding specifications have been improved significantly. Much of this improvement is based on the application of fundamental principles of thermodynamic and kinetic parameters which have been determined (Turkdogan and Fruehan; 1999).

2.1 Basic Oxygen Process

The oxygen converter process (LD/BOF and its derivatives) is a refinement step in the production of steel from ore. The main purpose of the process is to remove excess carbon from the pig iron produced in the blast furnace. The main feature of the process is to add oxygen through a top lance, in order to remove unwanted impurities through oxidation. It is the main method of carbon and low alloy steelmaking, annual production approaching to 60% of total crude steel production (Jalkanen; 2006). BOF is a widely preferred and effective steelmaking method due to its high productivity and considerably low production cost (Wang, Han and Wang; 2010). LD/BOF process consists of these subprocesses:

1. Charging slag
2. Charging hot metal
3. Oxygen blowing and addition of slagging and alloying additives
4. Measurement of steel temperature and composition
5. Tapping of steel
6. Tapping of slag

The first commercial operation of steelmaking with oxygen top blowing in the converter was in the early 1950s at Linz and Donawitz (Austria). This manner of steelmaking became known as Linz-Donawitz or LD process. For many years now, most of the steel has been made by top oxygen blowing for which different names are given. For example, in European steel plants the process is still called LD; in the UK, BOS (basic oxygen steelmaking); in the Far East and America, BOF (basic oxygen furnace), with the exception of U.S. Steel where it is called basic oxygen process (Turkdogan; 1996).

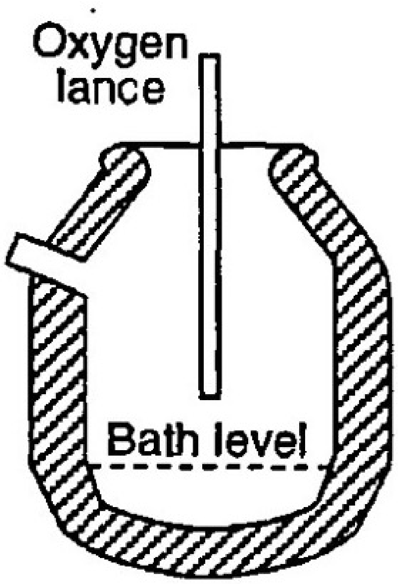


Fig. 2 – 1: Production of steel in the converter with top-blown oxygen (LD/BOF) (Turkdogan; 1996).

In the early 1970s, a bottom-blown oxygen steelmaking process was developed in Canada and Germany. This process, known as OBM in Europe and Q-BOP elsewhere, was in full size commercial operation by the mid 1970s in U.S. Steel plants followed by several plants in Europe and Japan. The tuyeres, mounted in a removable bottom, consist of a central pipe for blowing oxygen together with burnt lime, and an annular gap around the central pipe for the passage of gaseous hydrocarbon, e.g. propane or natural gas (Turkdogan; 1996).

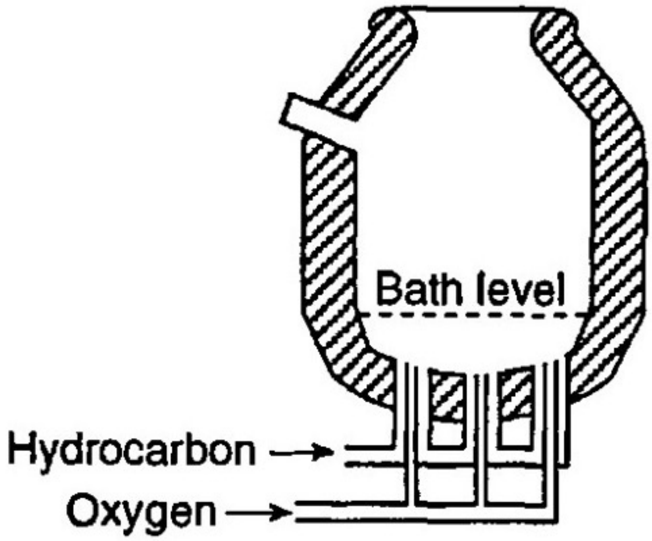
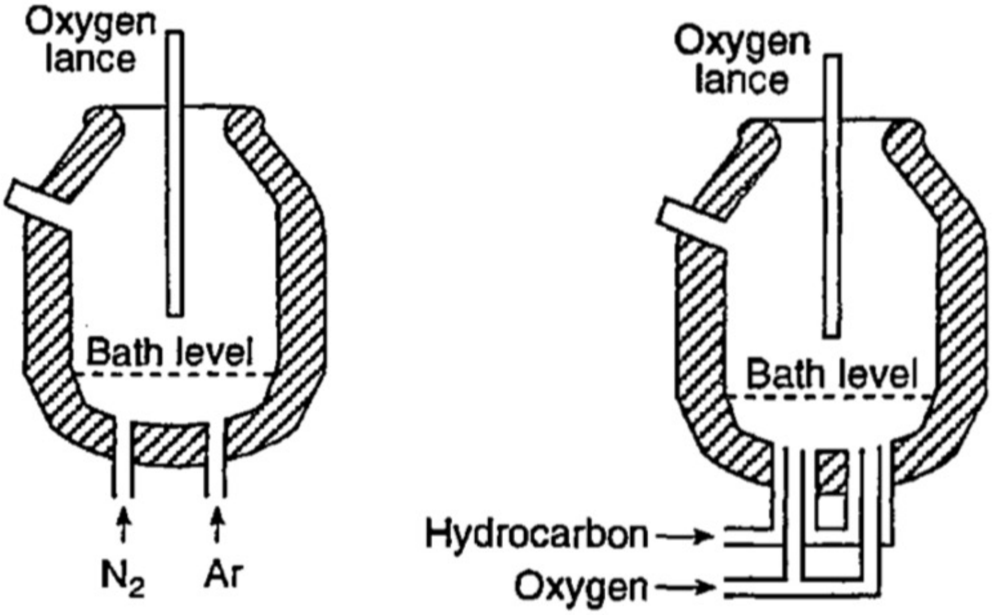


Fig. 2 – 2: Production of steel in the converter with bottom-blown oxygen (Q-BOP) (Turkdogan; 1996).

Further developments in oxygen steelmaking led to the present practices of various types of top and bottom blowing known as combined blowing. There is also post combustion of CO in the upper part of the vessel to generate additional heat for steelmaking (Turkdogan; 1996).

In modern steel mills about 300 tons of steel are produced within a 30-40 minute cycle. Various additives are added during the process to adapt the steel quality and slag formation. The converter furnace is inclined during charging and tapping. The converter has a vertical position during oxygen blowing. The changes in the position of the converter during the individual elementary processes are shown in the figure 2 – 4.

Depending on local operating conditions, availability of scrap, blast furnace iron and the extent of hot metal pretreatment, the metallic charge (LD/BOF, Q-BOP) is 75 to 95 % pig iron and the remainder is steel scrap. The types of scrap used are usually those produced in a steel mill: sheet scrap, damaged molds, bimetallic cans etc Turkdogan (1996).



(a) Combined LD/BOF. (b) Combined Q-BOP.

Fig. 2 – 3: LD/BOF a Q-BOP processes in oxygen convertor with combined blowing.

Oxygen is blown at a high speed (up to twice the speed of sound) on the surface of the metal bath in the converter and so-called hot area is formed in the region where the oxygen stream hits the surface. The oxidation products dissolve in the slag, with the exception of carbon monoxide, which passes through the slag layer and forms the major component of the converted gas. The oxidation intensity of the individual elements depends on their chemical affinity for oxygen. Carbon oxidation is one of the most important processes. Carbon is oxidized in the metal during the steelmaking process by the influence of oxygen, in particular on CO and partly on CO_2, depending on the reactions

$$C + \frac{1}{2} O_2 \longrightarrow CO \tag{2.1}$$

$$C + O_2 \longrightarrow CO_2 \tag{2.2}$$

Manganese is oxidized to MnO

Fig. 2 – 4: Representation of elementary processes in LD converter.

$$Mn + \frac{1}{2}O_2 \longrightarrow MnO \tag{2.3}$$

Phosphorus is undesirable in steel and oxidizes to P_2O_5

$$2P + \frac{5}{2}O_2 \longrightarrow P_2O_5 \tag{2.4}$$

Sulphur is a harmful element and passes into the slag in the form of CaS based on the reaction of CaO

$$CaO + MnS \longrightarrow CaS + MnO \tag{2.5}$$

whereby MnS is formed by reaction

$$Mn + S \longrightarrow MnS \tag{2.6}$$

and sulphur also goes out in the form of gas as SO_2

$$S + O_2 \longrightarrow SO_2 \tag{2.7}$$

Silicon has a high affinity for oxygen, so it is easily oxidized to form SiO_2

$$Si + O_2 \longrightarrow SiO_2 \tag{2.8}$$

In the initial stages of blowing, most of the silicon oxidizes to form a slag of low basicity - the composition of the metal and slag changes, as shown in the figure $2-5$.

An intense oxygen flow induces fluid flows in the iron bath, forcing the highly oxidized metal and the molten oxidation products from the iron bath surface to penetrate into the bath, where they react with the ”fresh” hot metal with a high content of impurities and therefore loss of iron in the form of FeO and Fe_2O_3 should also be considered:

$$Fe + \frac{1}{2} O_2 \longrightarrow FeO \tag{2.9}$$

$$2\,Fe + \frac{3}{2} O_2 \longrightarrow Fe_2O_3 \tag{2.10}$$

This oxygen stream and gas bubbles generated in the bath bring portions of the iron melt to the slag. The heat generated by the highly exothermic oxidation reactions is consumed by heating and melting the feed materials, heating the iron bath, slag and carbon oxides that are formed during the oxidation of the carbon and are partially lost to the environment during the blowing process.

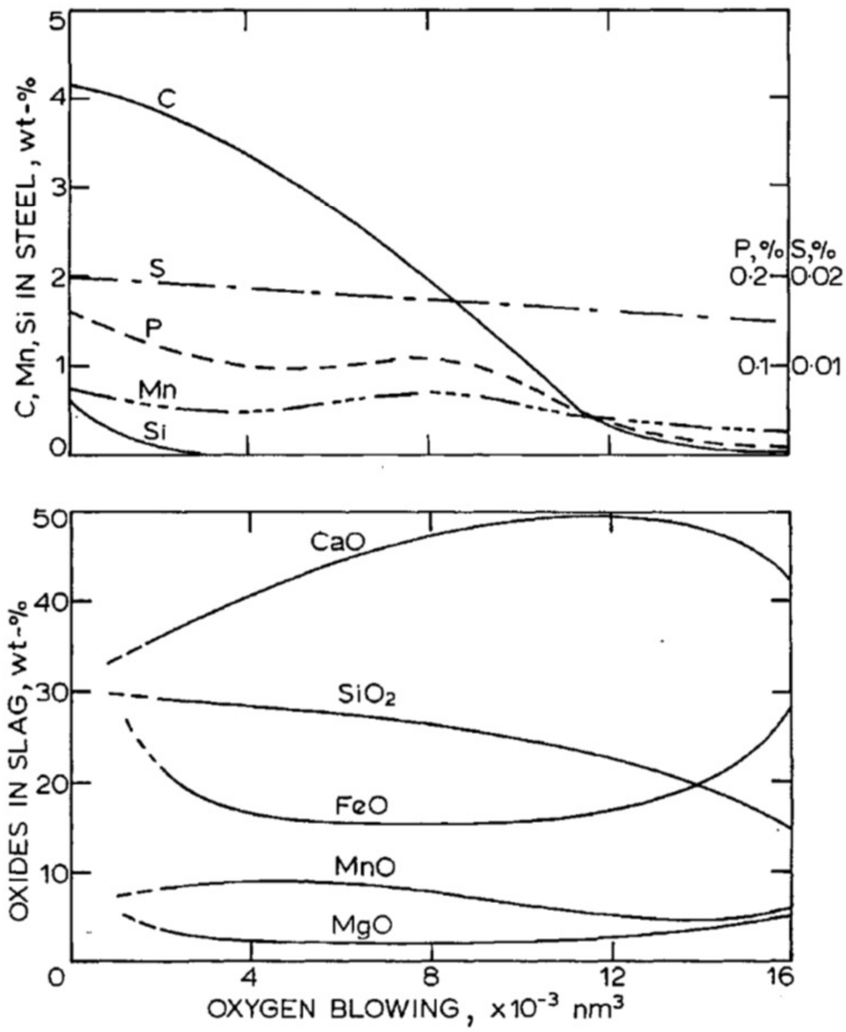


Fig. 2 – 5: Changes in metal and slag composition during steel production in LD/BOF process (Turkdogan; 1996).

The resulting SiO_2 passes into the slag as $2\,CaO \cdot SiO_2$ according to the equation

$$SiO_2 + 2\,CaO \longrightarrow 2\,CaO \cdot SiO_2 \tag{2.11}$$

and additionally, P_2O_5 passes into the slag as $3\,CaO \cdot P_2O_5$ according to the equation (Laciak et al.; 2017)

$$P_2O_5 + 3\,CaO = 3\,CaO \cdot P_2O_5. \tag{2.12}$$

Circulation in the iron bath caused by the flow of oxygen, rising gas bubbles and purging of inert gas through the lower tubes in converters with combined blowing type transports minor iron melt components (C, Si, Ti, Mn, P, V, etc.) to the upper bath layers (Jalkanen; 2006).

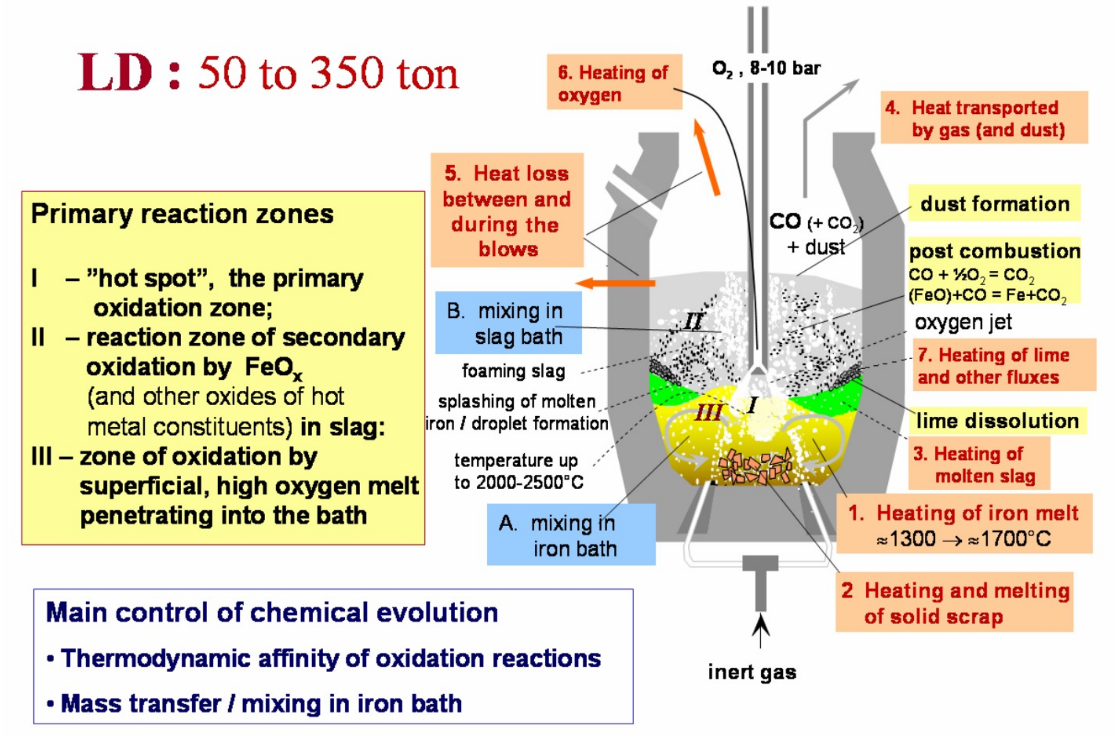


Fig. 2 – 6: Chemical and thermal processes in LD converter (Jalkanen; 2006).

In order to monitor and control the process, different measuring systems can be employed to give feedback to either the operator or directly to existing system for automated control. These measurements can be either direct or indirect as well as with or without time delays. The real-time information on the process state can be obtained from a number of sensors, e.g. off-gas flow rate from venturi; off-gas temperature with temperature sensors; indication of changes in slag level from sound level measurement with microphone, accelerometer on lance or vessel or lance elongation sensor; pressure difference with ambient pressure with hood pressure sensor, etc.

All these signals can, in principle, be used for closed-loop control. Changes in lance height are easier to measure as well as set and therefore preferable to use in a closed-loop control system. Oxygen gas flow rate should not be changed more than approximately $\pm 5\%$ since the nozzle is designed for a specific flow rate (Widlund et al.; 1998). System architecture for closed-loop control of basic oxygen steelmaking is described in a schematic representation in Fig. 2 – 7.

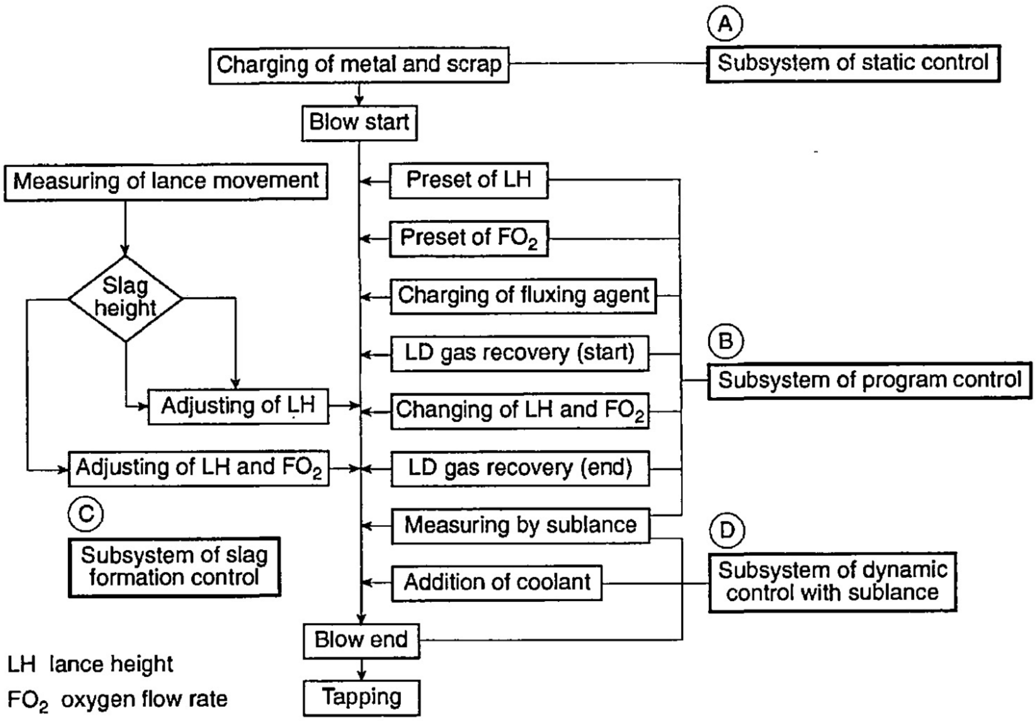


Fig. 2 – 7: Schematic representation of the system and function of fully automatic LD/BOF process (Turkdogan; 1996).

Different operators apply different rules for deciding when to stop the blowing of oxygen. These operator induced irregularities make it difficult to achieve production disturbances. The converter process is only one link in a chain of unit operations from raw materials to final product. Therefore, production disturbances can change process conditions. For example, poor blast furnace performance might lead to insufficient hot metal supply or even production disruptions. Under these circumstances, more metal scrap and fuel should be used instead of hot metal to uphold production volumes. Logically, this implies changes in blowing practice (Widlund et al.; 1998).

2.2 Computer-aided Mathematical Modeling and Numerical Simulation

The motivation for using computer simulations to investigate metallurgical processes is two-fold. First, it enables design changes to be tested before building a prototype, which naturally leads to a lower total design cost. Second, it makes it possible to investigate phenomena that cannot easily be measured or observed in the process. Even a seemingly simple operation such as the continuous measurement of the temperature during the decarburization process is difficult due to the very high temperatures in the process and generally harsh conditions prevailing in the steel plants (Ersson and Tilliander; 2018).

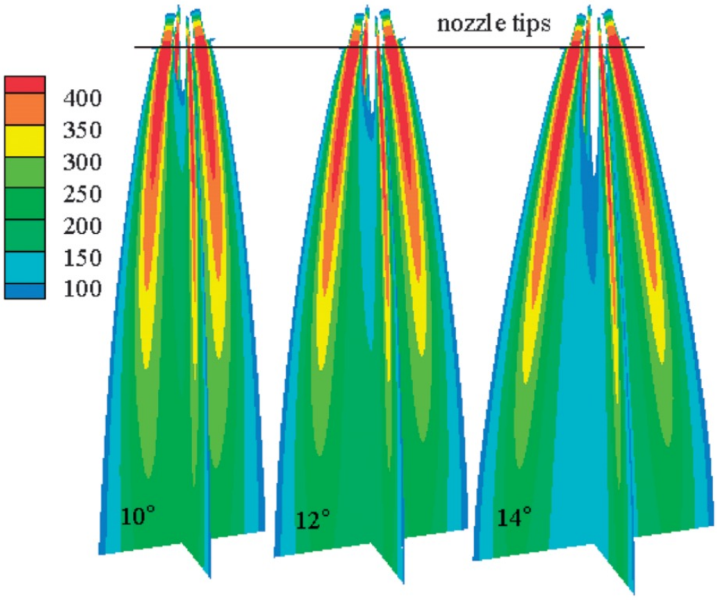
In metallurgy, simulating linear and non-linear processes that we encounter in steelmaking by creating mathematical models is of great importance. Since first attempts to use mathematical techniques for the simulation and optimization of large scale metallurgical operations (Ray et al.; 1973), various numerical methods were implemented as algorithms and used to simulate phenomena in steelmaking processes. One class of such methods is Monte Carlo, which is useful for simulating systems with many coupled degrees of freedom such as fluids.

Modern fluid mechanics problems would be impossible to solve without use of Computational Fluid Dynamics (CFD), since the scope of analytical solutions to fundamental equations of fluid mechanics is very limited and, once a more difficult geometry is encountered, we usually have to choose a given numerical method for obtaining a solution. CFD encompasses a wide spectrum of numerical methods used for solving complex three-dimensional (3D) and time-dependent flow problems (Rapp; 2017). Since early pioneering work in the metallurgical field done by Szekely et al. (1977), the cost of performing computer simulations has decreased over the last few decades, while the available processing power has increased. Most of the processors and processing units that are currently developed and produced have several cores that can execute instructions in parallel. Thus, the processing power available to a CFD software also depends on the capability of the software to execute in parallel. A study by Ersson and Tilliander (2018) of the last two decades of metallurgical CFD simulations reveals huge improvements on the type of phenomena that can be explored and we will see this trend is continuing thanks to improvements in both the available processing power and the available algorithms. Therefore CFD found its way into numerous studies in steelmaking, where these methods proved useful in demonstrating the hidden and significant properties. However, its use in the steel industry may not be as integrated as in the aero and automotive industries, in which the development of new designs is of key importance. The major difference between aero and metallurgical industries is that the metallurgical industries almost always deal with multiphase systems at elevated temperatures and that the motivation of modeling is mainly process optimization. With a continuing development in multiphase models as well as in reacting flow modeling, the continued usefulness of CFD in metallurgy remains clear.

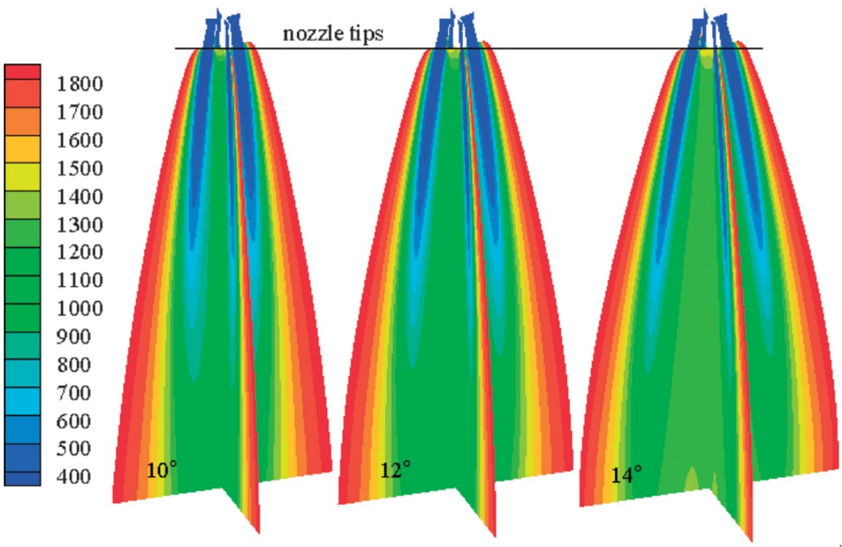
In LD/BOF process, different chemical reactions among oxygen, slag, and molten iron in oxygen converter, in combination with vigorous stirring process to promote slagging, dephosphorization, decarbonization, heating of molten steel, and homogenization of steel composition and temperature, determines the final properties of steel. The objective of the oxygen converter is to refine molten iron to crude steel through oxidization to achieve a specified temperature and chemical composition at the end blow. Failure to do this leads to the need to reblow. The impact of oxygen jet into molten bath strongly affects the bath and promotes the three-phase flow among gas, slag, and molten steel in the bath. With the move from old rule-based systems to a model-based, real-time closed-loop control of lance movement and oxygen flow, significant drawbacks were eliminated. There have been efforts in developing accurate and efficient numerical models within CFD field to solve the jets flow in the oxygen converter. Peng and Han (1996) established the conditions of optimum nozzles of performance by deriving the system of mathematical equations to simulate the steady, quasi-one-dimensional supersonic flow through a single De Laval nozzle. Tago and Higuchi (2003) analyzed single-nozzle and multi-nozzle lances with the help of two-dimensional simulation based on fluid dynamics and found that higher ambient temperature leads to the lower density and the higher velocity of the gas jets, but does little affect the dynamic pressure. They report that CFD proved useful method to predict the effect of the inclination angle and the number of the nozzles on the jet behavior in the top blown processes. Wang, Yuan, Matsuura, Zhao, Cheng and Tsukihashi (2010) developed a three-dimensional mathematical model to simulate the compressible jets flow from the top-blown lance, taking into consideration variations of fluid density, viscosity, high temperature and Mach number. They demonstrated that k–ω turbulence model is superior to the widely used k–ε turbulence model to calculate turbulent conditions within multiple jets. Simulation results of final computational flow field distributions of three kinds of multiple jets are shown in Fig. (2 – 8).

CFD models have been also used in developing deeper understanding of the decarburization processes in steelmaking. However, these processes are highly complex with large variations in time and length, and therefore it makes the systems extremely demanding to simulate. Ersson and Tilliander (2018) reviewed latest research on the subject from 1998 until 2016 and found out that, even though several reports have been published discussing research about modeling parts of the decarburization processes numerically, no models have been presented that can handle the entire complexity of the processes. Many authors had simplified the system in existing models in order to achieve an understanding of particular phenomena rather than of the entire process.

Another important part of the oxygen steelmaking process is keeping the usual balance of 80% hot metal and 20% scrap during charging to regulate the temperature of steel in the



(a) Velocity magnitude (m/s)



(b) Total temperature (K)

Fig. 2 – 8: Simulating results of velocity magnitude and total temperature field distributions of the three kinds of multiple jets: (a) velocity magnitude (m/s) and (b) total temperature (K) (Wang, Yuan, Matsuura, Zhao, Cheng and Tsukihashi; 2010).

vessel. To define the charge conditions and oxygen blowing requirements to achieve the temperature and chemical composition, mathematical and thermodynamic models have been developed (Kačur et al.; 2019; Laciak et al.; 2018). Reactions that take place in LD process can vary significantly from heat to heat, while not many variables involved are not accurately known. Therefore, it is necessary to take into account the uncertainty affecting the whole process reactions. To correct the differences between the theoretical predictions of the process models and the real results, Bouhouche et al. (2012) introduced a random quantity term into their models and improved the prediction model with the use of Support Vector Regression and Monte Carlo Simulation methods in combination. Most of the control schemes rely on an accurate system model. However, as these systems become more complex, writing down the dynamics from the first principles is extremely challenging. In such cases, neural networks are used to approximate the dynamics directly using system data. In this context, neural networks can be thought of as a generalization of linear regression for non-linear dynamics. At the Institute of Control and Informatization of Production Processes at BERG Faculty (TUKE), team around Laciak et al. (2018) built upon Bouhouche's work and started experimenting with machine learning in process control and its application in oxygen steelmaking, precisely in LD converter. They applied Support Vector Machines (SVM) and Support Vector Regression (SVR) to predict the final melt temperature and final carbon concentration based on dynamical data. Their work also focuses on developing innovative fractional-order mathematical models for indirect measurement of molten steel temperature and concentration of CO and CO_2. The non-linear nature of these processes presents the opportunity to model them by using derivatives of non-integer order, which in their definition are based on the influence of past data on the present value of derivative.

In some simplified form, combinations of numerical simulations and visualizations of steelmaking processes can be used as a educational tool in process control courses at technical universities. The aim of the online, web-based interactive simulation of basic oxygen steelmaking at steeluniversity.org shown in Fig. 2 – 9 is to introduce students to this process in a more fun and engaging way.

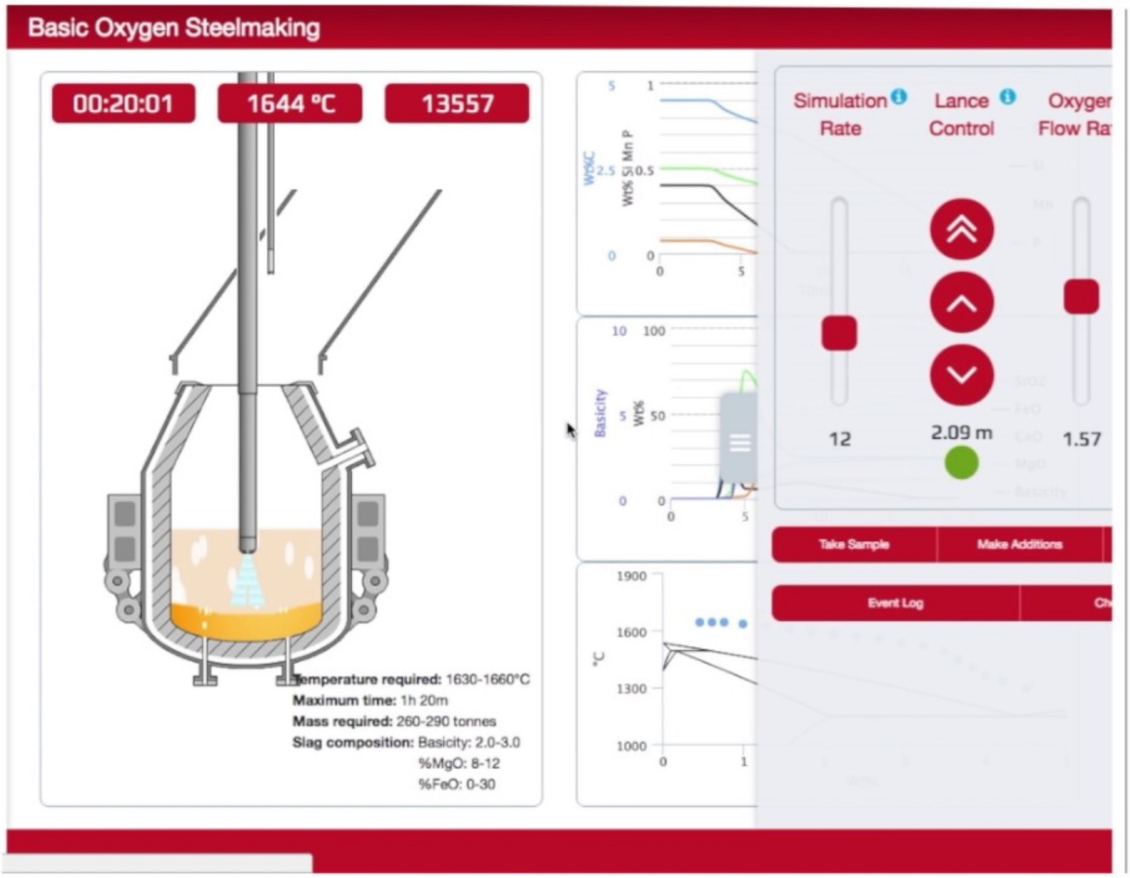


Fig. 2 – 9: Interactive, educational simulation of basic oxygen steelmaking by steeluniversity.org.

2.3 Process control

The need for developing improved control systems has traditionally been powered by the demand for more accurate and cost efficient production. This is still a major driving force but environmental issues do also have a profound influence on this development today (Widlund et al.; 1998).

The main objective of controlling oxygen converter steelmaking is to obtain prescribed parameters for the steel when it is tapped from the furnace, including weight, temperature, and each element content. In practical steelmaking process, the criterion whether the molten steel is acceptable or not is often decided by the endpoint carbon content and temperature (Wang, Han and Wang; 2010).

Generally, the LD/BOF steelmaking process with sub-lance system can be divided into two stages: static control and dynamic control. Static models include oxygen supplying model, slaging model and bottom blowing model; dynamic models include decarburization speed model, molten steel warming model and the model for the amount of coolant. (Wang, Han and Wang; 2010).

The fast dynamics of the LD converter steelmaking process or the BOF process, as it is commonly known, often makes it a challenge to obtain stable blowing conditions and to achieve the required steel composition and temperature simultaneously at the end point. For this reason, process control becomes very necessary and attempts had started as early as in the 1970s (Fritz and Gebert; 2005). Out of the originally very simple LD process have grown the modern process-controlled and automated production systems that enable present-day adaptations to meet today's economic and ecological demands (Sarkar et al.; 2015). The non-linear nature of chemical and thermodynamical processes in basic oxygen steelmaking also amassed interest in developing new mathematical models based on fractional-order calculus.

2.4 Visualization and Virtual Reality

Scientific visualization is the use of computer graphics to create visual images that aid in the understanding of complex numerical representations of scientific concepts or results. Computational fluid dynamics (CFD) based numerical simulations often output massive amounts of data. These simulations often contain high-dimensional data in a three-dimensional volume. The display of phenomena associated with this data may involve complex three-dimensional structures.

Non-immersive interactive visualization systems implemented for the conventional desktop and mouse are effective for moderately complex problems. Kealy and Subramaniam

(2006) defines mouse-based interactivity type of virtual reality as ”virtual realia”. Milgram et al. (1994) puts forward and idea of ”virtuality continuum” in his Extent of Presence Metaphor, where he states that virtual realia type of desktop virtual reality visualization is essentially a ”window-on-the-world” with a fixed monoscopic viewpoint; changes in the viewer’s head position do not result in different perspectives of the object.

Immersive virtual environments, by comparison, lie at the other end of the spectrum and permit looking around an object by moving one’s head position. Therefore, a fundamental difference between desktop-and-mouse virtual realia and immersive VR is that the latter is a true 3D representation that may be either viewer or object-centered while the first is exclusively viewer-centered. In other words, changes in the relative positions of a 2D object’s components result from shifts in the viewer’s perspective. The same may be true for objects viewed in a three dimensional environment, whether real or virtual. However, in such an environment, an object may also appear to change shape (e.g., through foreshortening), not due to an altered position of the viewer, but because the object itself has moved to a different position. Immersive virtual reality displays aid in the unambiguous display of these structures by providing a rich set of spatial and depth cues. Virtual reality interface concepts allow the rapid and intuitive exploration of the volume containing the data, enabling the phenomena at various places in the volume to be explored, as well as provide simple control of the visualization environment through interfaces integrated into the environment (Bryson; 1996).

Desktop-and-mouse interfaces for 3D visualizations make it difficult to specify positions in three dimensions and do not provide unambiguous display of 3D structure. Virtual reality interfaces attempt to provide the most anthropomorphic interfaces possible - that means they must be human-conforming and should be designed to allow the most natural, unambiguous way of scientific exploration. They must include two components: display and user control. Scientific visualization makes particular demands on virtual reality displays. The phenomena to be displayed in a scientific visualization application often involve delicate and detailed structure, requiring high-quality, high-resolution full-color displays. A wide field of view is often desirable, because it allows the researcher to view how detailed structures are related to larger, more global phenomena.

Historically, the early attempts at using head-mounted virtual reality technologies started with CRT-based Binocular Omni-Oriented Monitor (BOOM) created by Fakespace Systems Inc. BOOM was a stereoscopic display device with screens and optical system housed in a box that is attached to a multi-link arm. Head tracking was accomplished via sensors in the links of the arm that holds the box.

Advent of commodity-level VR hardware like HTC Vive or Oculus Touch has made this technology accessible for meaningful applications. These headset utilize lasers and photosensitive sensors (HTC Vive) or cameras (Oculus Touch) for head and hands tracking and provide six degrees of freedom (6DoF) for movement in virtual environment. By immersing the user into the simulation itself, virtual reality reveals the spatially complex structures in computational science in a way that makes them easy to understand and study. But beyond adding a 3D interface, virtual reality also means greater computational complexity (Bryson; 1996). The ability to provide real-time interaction can provide strong depth cues, either through allowing interactive rotations or through the use of head-tracked rendering. Applications and techniques are being developed to discern how immersive technology benefits visualization. The medical field provides an especially promising context for this development, as medical practitioners require a thorough understanding of specific 3D structures: human anatomy. Users may interact simultaneously with high resolution computed tomography (CT) scans and their corresponding, 3D anatomical structures.

Another frequently used type of immersive, interactive display technology nowadays is projection-screen-based Cave Automatic Virtual Environment (CAVE). These systems consists of 3 to 6 large displays positioned into a room-sized cube around the observer. The walls of a CAVE are typically made up of rear-projection screens, but recently the flat panel displays are commonly used. The floor can be a downward-projection screen, a bottom projected screen or a flat panel display. The projection systems are very high-resolution due to the near distance viewing which requires very small pixel sizes to retain the illusion of reality. The user wears 3D glasses inside the CAVE to see 3D graphics generated by the CAVE. People using the CAVE can see objects apparently floating in the air, and can walk around them, getting a proper view of what they would look like in reality. This is made possible by infrared cameras. Movement of the observer in the CAVE is tracked by the sensors typically attached to the 3D glasses and the video continually adjusts to retain the viewers perspective.

Many universities and engineering companies own and use CAVE systems. Researchers can use these systems to conduct their research topic in a more effective and accessible method. Engineers have found them useful in enhancing of a product development through prototyping and testing phases.

For technical sciences, mathematics is an important part of the university curriculum. The study of Kaufmann et al. (2000) utilized Construct3D, a three-dimensional geometric construction tool based on the collaborative augmented reality system Studierstube to educate users in mathematics and geometry. By working directly in 3D space, complex spatial problems and spatial relationships may be comprehended better and faster, because students had to calculate and construct mathematical objects and relationships between them with traditional (mostly pen and paper) methods. Their system utilized a stereoscopic head-mounted display and the Personal Interaction Panel, a two-handed 3D interaction tool, and found that the use of VR technology in the form of Construct3D facilitates ease of learning and encourages experimentation with geometric constructions.

In field of mathematics, VR application named Cal (2019) is making serious progress. It is developed by a company *Nanome, Inc.* started by students from University of California San Diego. Team behind Calcflow is using VR to help students grasp the biggest ideas in vector calculus. Its features include visualizations of vector addition, cross product, parametrized functions, spherical coordinate mapping, double and surface integrals. Beside Calcflow, they are implementing a VR platform specialized for atomic, molecular and protein visualization, built for researchers and scientists (Nan; 2019). Interactions can play a crucial role in increasing learner engagement, if designed appropriately. VR tools, methods, procedures and affordances of a virtual world can lead students into having meaningful and engaging conversations (Christopoulos et al.; 2018). A variety of visualization techniques can be used to see and understand various graphical representations of mathematical functions through location, shape, color, and even animation of a resulting visual object (Kaufmann; 2011). One can say that virtual reality established itself in many disciplines of human activities, as a medium that allows easier perception of data or natural phenomena appearance.

In fact, theme of this dissertation was influenced by my previous work with using virtual reality for mathematics education at the university. Focus of my masters thesis was on studying if the immersiveness and interactivity in VR was helpful for studying complex themes in mathematics. I have created web-based virtual reality (WebVR) application called MathworldVR, which explored the possibilities and limits of web technologies for creating room-scale, immersive, virtual learning environments (VLE) for helping students to explore, learn about and experiment with various parametrized functions. Main benefit lies in that it provides an intuitive ways of instrumental interaction by using direct visual manipulation of the input variables, which shortens the time for learner to understand underlying principles of given mathematical subject. It is also a practical tool for teachers to create visualizations and showcase abstract concepts in concrete 3D environment during lectures (Fig. 2 – 10).

It was influenced by our previous work on web-based, 2D and 3D visualizations and interactive apps that provided an aid for teaching mathematics at Technical University of Košice (Pócsová et al.; 2016; Pocsova et al.; 2019). Output of our work was set of online presentations with solved examples of parametrized functions, containing 3D graphs with representation of partial derivatives, stationary points and steps of the functional analysis (Fig. 2 – 11). The use of interactive visualizations and animation techniques showed potential in classroom but also outside of it. Our work showed that visualization is essential for understanding not only complex processes but also things like quantum computation.

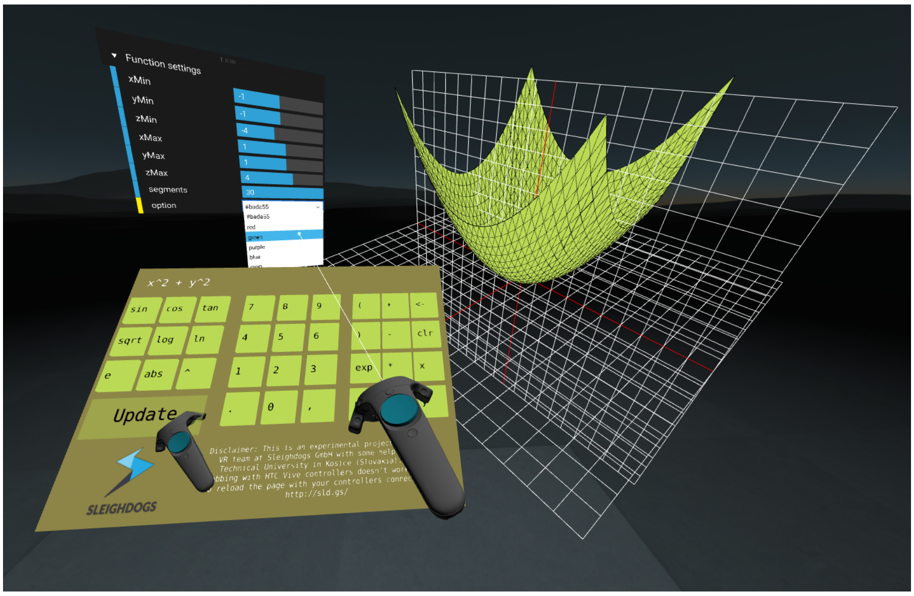


Fig. 2 – 10: MathworldVR immersive VR environment viewed through head-mounted display with graphical interface that user interacts with by using hand controllers.

Researchers Lin et al. (2018) from Zhejiang university created QuFlow - an application for visualizing parameter flow in quantum circuits for understanding quantum computation. Work like this is crucial for development of new algorithms for quantum computers.

Substantial amount of work in applying 3D visualizations and virtual reality for solving technological issues and bringing new trends into steelmaking industry is currently happening at Center for Innovation through Visualization and Simulation (CIVS) at Purdue University Northwest (located in Indiana, USA). CIVS has been globally recognized for its integrated and application-driven approaches through state-of-the-art simulation and virtual reality visualization technologies for providing innovative solutions to solve various university research problems, industry issues, as well as education. More than 350 projects that have been completed at the center from its inception in 2014 until today provided substantial educational and economic impact, resulting in more than 40 million US dollars (more than 36.1 million € at the time of this writing) in savings for companies. In collaboration with other universities and companies from steelmaking industry, they focus on research regarding integration of virtual reality with simulation technologies

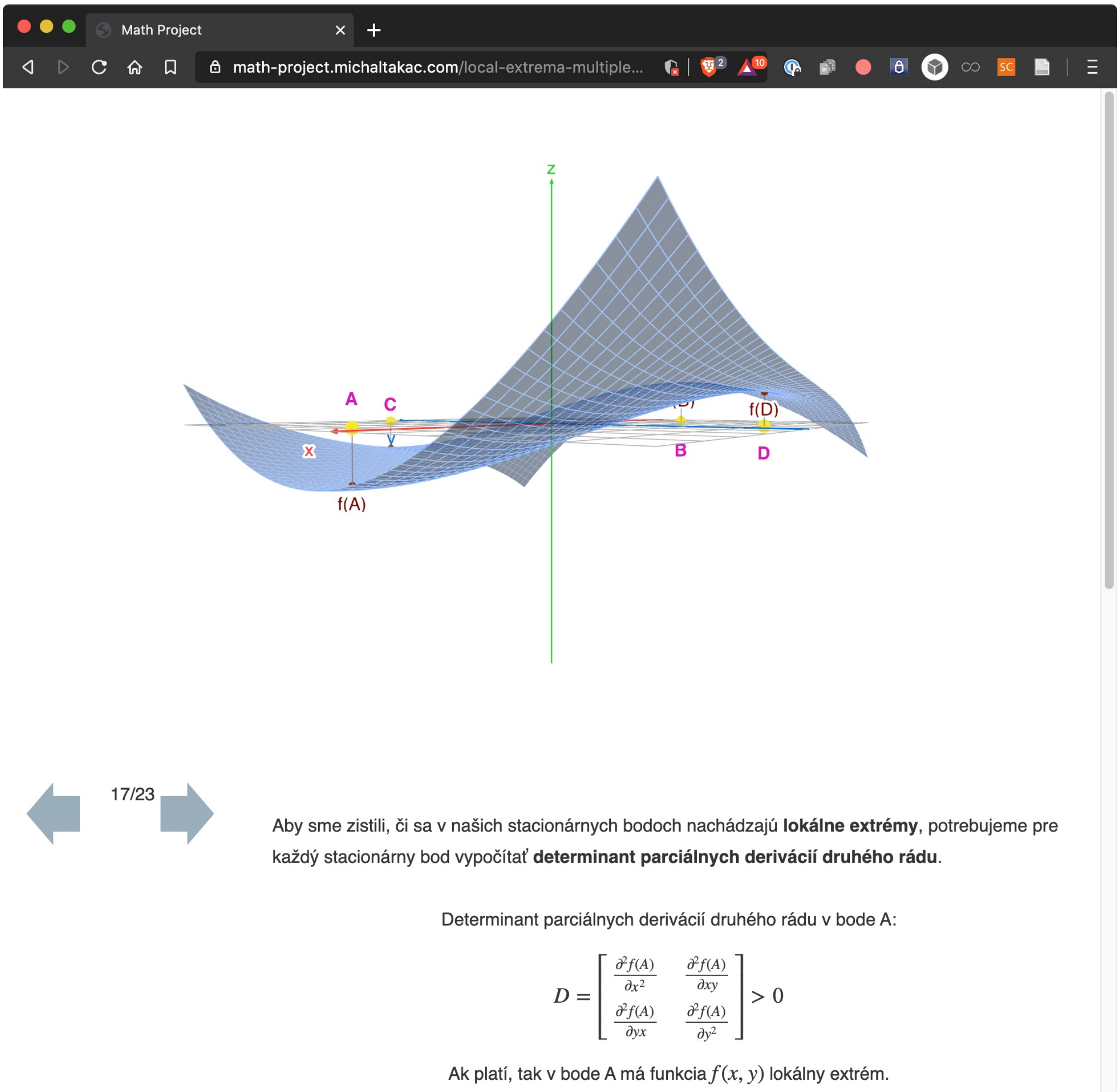


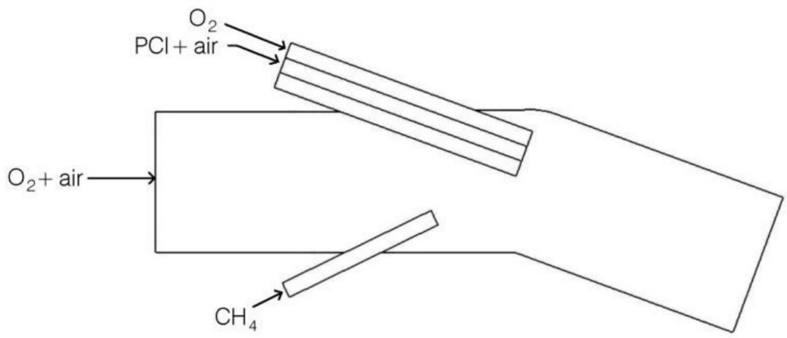
Fig. 2 – 11: Interactive online presentations as an aid for teaching mathematics at Technical University of Košice.

and high performance computing; application of simulation and visualization technologies to industrial processes for process design trouble-shooting and optimization to address the issues of productivity, energy, environment, and quality; and last but not least, development of advanced learning environments in virtual reality for training and education. With funding support provided by a major AMTech grant from the U.S. Department of Commerce, they launched novel, industry-led association of steel manufacturers and stakeholders called Steel Manufacturing Simulation and Visualization Consortium (SMSVC).

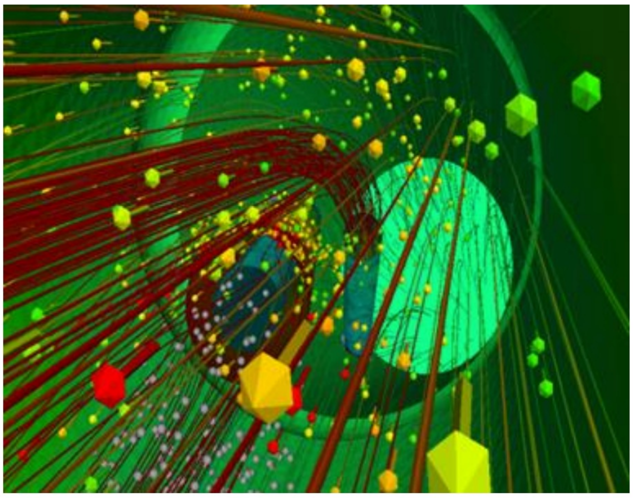
Interesting application of combining 3D CFD smulation and virtual reality for visual inspection is pulverized coal injection (PCI) and coke combustion model. Research efforts between the Canadian government (CANMET), CIVS and the American Iron and Steel Institute (AISI) were conducted and resulted in modeling of the blowpipe and tuyere of the blast furnace. Combination of aforementioned technologies turned out to be powerful and provided detailed information of flow streams that were previously very difficult to measure. The CFD model shown in Fig. 2 – 12 was used to simulate PCI with natural gas co-injection in the lance, blowpipe and tuyere.

Effects of operating parameters such as blast temperature, natural gas flow rate, oxygen enrichment, and PCI carrier air rate were further investigated. Results form the simulation informed further realization to stop cold oxygen flow incection through the oxy-coal co-axial lance. The outcome was significant downtime avoidance due to fewer failures of penstock and fuel lances. This process change realized a coke savings of 15 lbs/NT hot metal that resulted in a yearly potential cost avoidance of 8.5 million US dollars at full production.

Another very interesting project conducted at CIVS involved development of comprehensive package of modules for simulating multiple processes in blast furnace. 3D CFD model shown in Fig. 2 – 13 has been developed by Zheng and Hu (2014) specifically for simulating the blast furnace hearth. The campaign life of a blast furnace is highly dependent on residual thickness of refractory lining in the hearth. The progress of hearth lining erosion is greatly affected by hot metal flow patterns and heat transfer in refractory under different operating conditions. CFD model incorporates both the hot metal flow and conjugate heat transfer through the refractories. They achieved consistency of results between measured and calculated refractory temperature profiles, as the model has been extensively validated using measurement data from industry blast furnace. The virtual reality (VR) visualization technology has been used to analyze the velocity and tempera-



Schematic of the injection system



Temperature distribution inside the injection system

Fig. 2 – 12: CFD simulation of pulverized coal injection system.

ture distributions and wear patterns of different furnaces and operating conditions. This interactive 3D visualization is shown in Fig. 2 – 14. Based on the results, it was possible to predict the inner profile of hearth and provide guidance to protecting the blast furnace hearth.

Part of the project is also complex set of numerical simulations of various processes in blast furnace combined into interactive and immersive 3D models viewable through VR headsets or explorable in CAVE systems. Fig. 2 – 15 describes some of the simu-

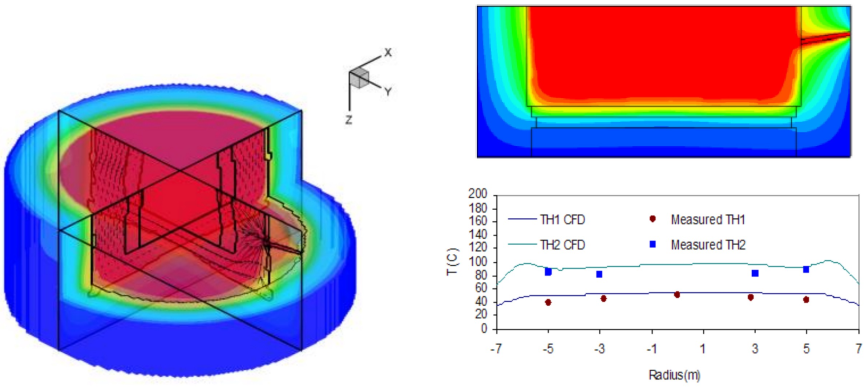


Fig. 2 – 13: CFD model for simulation of temperature distribution in blast furnace hearth.

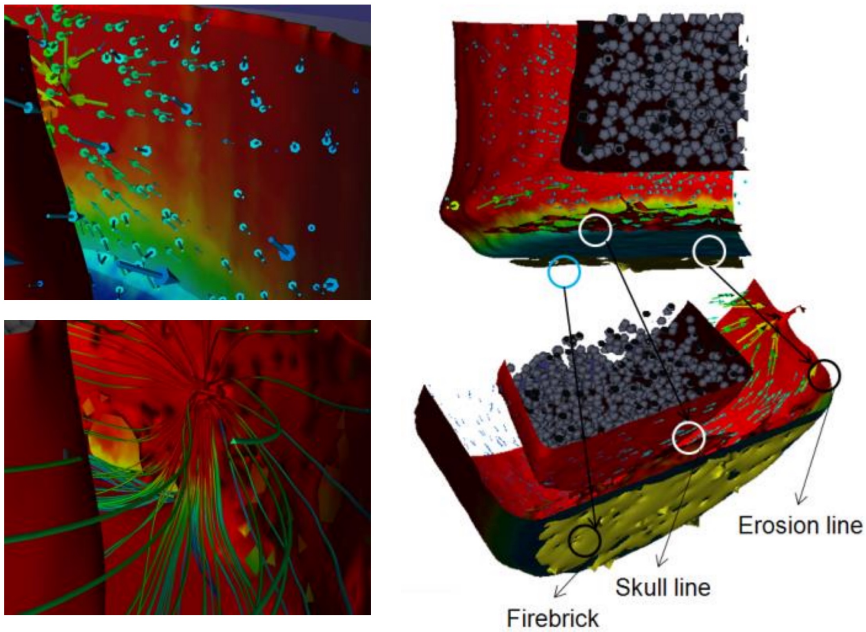


Fig. 2 – 14: 3D visualization of CFD results using CAVE-based VR system.

lation packages and Fig. 2 – 16 shows gas and burden distribution visualization of CFD simulation inside blast furnace shaft.

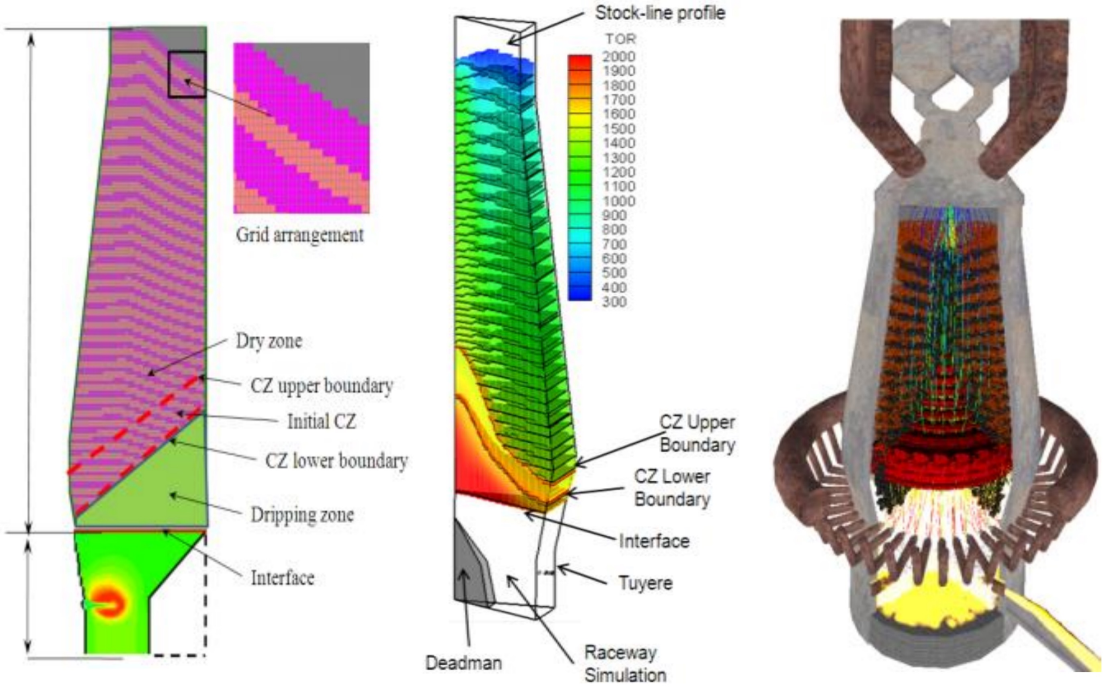


Fig. 2 – 15: Blast furnace simulation and visualization.

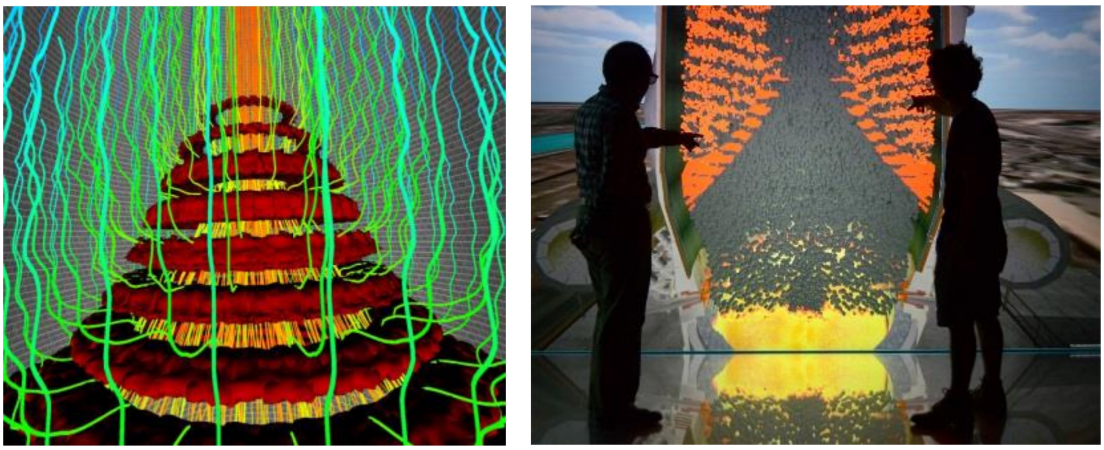


Fig. 2 – 16: 3D visualization of gas and burden distribution inside blast furnace shaft.

3 Proposed Methodology

This dissertation thesis deals with design and implementation of modern methods in process control. Since I have been consulting and working professionally with virtual reality and at the Institute of Control and Informatization of Production Processes, where significant work has been done in steelmaking field with focus on basic oxygen process (LD/BOF), I've decided to focus my attention to using VR technology and interactive 3D graphics for modeling, simulating and optimizing the LD/BOF process. I've been in close contact with other researchers that have hands on experience with research in this area (Kačur et al.; 2019; Laciak et al.; 2018) which provides me with the much of the needed consultations, further contact with steelmaking industry companies in Košice and central European region, and data gathered from numerous studies.

As research studies and projects implemented at CVIS shown, new trends like high-resolution 3D simulation and VR technology can be largely helpful in optimizing metallurgical processes. Immersive VR simulations of blast furnace presented in previous section has clearly shown the potential of these technologies and delivered significant economical impact. As vast majority of steel manufactured in the world is produced using the LD/BOF process, similar approaches should be considered and tried as for the blast furnace mentioned above in section 2.4.

Static, high-quality 3D representation of LD converter will be modeled, with walls and inner parts each modeled separately, so the 3D model is modular enough for further work that involves composing static and dynamic parts together. Work on this phase was already started, with design and 3D modeling of basic oxygen furnace (LD converter) based on models from steeluniversity.org in open-source, 3D modeling software, Blender. In the meantime, discussions about possible collaboration with SteelUniversity has been initiated with the goal of taking advantage of already existing static 3D models like the one shown in Fig. 3 – 1.

3D simulations of chemical and thermodynamical processes in basic oxygen steelmaking

Fig. 3 – 1: Annotated model of LD converter with information about each part that can be displayed by clicking on the numbers (created by steeluniversity.org and hosted on Sketchfab). It has been created for educational purposes.

will be created with use of computational fluid dynamics (CFD) methods. CFD software like ANSYS, SimScale and OpenFOAM will be analyzed and most suitable one picked for creation of aforementioned simulations. Special attention will be placed on interactivity features and how visual exploration of final simulations can be achieved. Interactivity of 3D models and manipulation of simulation time scales is of great importance.

Immersive environment in virtual reality will be designed and implemented in Unity and Unreal Engine software. It will be designed to be used in conjunction with off-the-shelf, commercial, six-degrees-of-freedom (6DoF) VR headsets, hand controllers and hand trackers. It will include combination of static 3D models of LD converter (in different variations e.g. with varied opacity of the walls or bisected) with dynamic, interactive inner part consisting of 3D multi-phase CFD model simulating chemical and thermodynamical processes. These will be viewable separately or in combination according to user's preference. Impact of provided immersiveness to deepening of the understanding of various known processes and searching for hidden issues presenting themselves through simulations in this setting will be studied and analyzed.

Novel interactive 3D graphical interfaces for multi-phase virtual reality simulation will be designed and implemented. Hand and finger tracking will play important role in design of these interfaces. Users should be able to step into the live 3D simulation, use their hand as a pointer to get immediate feedback and information like slag temperature by pointing the laser ray from their hand at any point on the top of the slag or manipulate the time scales of the simulation by moving the slider on a timeline (inspired by time-travel debugging techniques utilized in game development and novel programming tools).

Possible by-product after finalization of previous objectives is the educational use of tools that will be created as a part of this dissertation. Relatively small tweaking of the software created would be needed to build a separate tool for training purposes of future converter operators, or in a more general way as a educative tool at technical universities.

4 Objectives of Dissertation Thesis

The proposed objectives of dissertation thesis are as follows:

1. Analysis of the current state of the art of modeling using modern methods.
2. Design of a suitable method for creating mathematical models of processes and their visualization in the VR environment.
3. Creation and implementation of supporting models and environment in VR.
4. Selection of technological process and design of appropriate CFD model.
5. Synthesis of created CFD model with VR environment.

5 Tézy dizertačnej práce

Navrhované tézy dizertačnej práce sú nasledovné:

1. Analýza súčasného stavu tvorby modelov s využitím moderných metód.
2. Návrh vhodnej metódy na vytváranie matematických modelov procesov a ich vizualizáciu v prostredí VR.
3. Vytvorenie a implementácia podporných modelov a prostredia vo VR.
4. Výber technologického procesu a návrh príslušného CFD modelu.
5. Syntéza vytvoreného CFD modelu s prostredím VR.

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