OPEN-SOURCE COMPUTING TOOLS FOR THE REFRACTORY ENGINEER OF THE PRESENT AND THE FUTURE

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ABSTRACT

Technology advances over the last century were able to reshape the world we live in. Relationships have been physically and virtually changed by innovations ranging from transportation (engines, airplanes) to communication, (with phones, the Internet, and satellites). Considering this, the abilities and skills required for young professionals have been changing dramatically, and the refractory industry has demanded an understanding of this new world and ability to solve its challenging problems. Due to the complexity of materials knowledge, which includes the latest advances in modeling and data science, a sophisticated blend of fundamental concepts and advanced techniques that challenges how to promote education effectively, has arisen. For instance, heat transfer mechanisms within the refractory material can be both discussed on the fundamental level or on how to carry out advanced simulations to describe it, giving the engineer the ability to solve real-life problems. The present work aims to classify this new set of needed tools, explore options to conciliate fundamentals with advanced tools and conjecture strategies to educate present and future professionals. As a conclusion, the minimum package of skills is presented considering the association of industry, academics, students and computing, all synergistically working together to solve the new challenges and induce innovation.

Introduction

Refractories are a category of materials able to withstand challenging conditions, ranging from high temperatures, high chemical activity and thermomechanical loads[1].

Current worldwide efforts to minimize the environmental impacts of human activities[2] adds a new dimension to the area of refractories: besides sustaining their function in harsh environments, the high- temperature ceramics must also do so with minimal carbon footprint and the highest possible energy efficiency by diminishing thermal losses, for instance[3]. Simultaneously, the advent of the Internet developed a scenario where collaboration can be made from a myriad of places. This also increased accessibility, rising to learning challenges such as finding the required information and filtering out valuable resources.

Thus, the traditional advanced techniques based on laws of physics that enabled complex models and simulations of different scenarios are now carried out by machine learning (ML) methods. These new algorithms are able to learn hidden patterns on the data that ranges from social media to the numerous parameters controlling a blast furnace, for instance. Today, the lack of transparency on how such algorithms take specific decisions is one of the greatest drawbacks of these methodologies. However, one should consider that the rapid growth of machine learning applications is carried out at a pace even greater than its fundamental understanding. As Dijkgraaf proposed, the main challenge of ML is to surpass its current black-box stage and finally lead to a deeper understanding of the world, just as alchemy once was the precursor to modern chemistry[4].

In this context, the present study aims to propose how the current required challenges in refractory innovations can be developed by linking the fundamentals to the digital tools, which could be critical for the new generations of refractory engineers. After providing an overview of the tools and proposing a roadmap for the refractory engineer of the present and the future, two illustrative examples are given in common areas of development and research of refractories materials: (i) the 3D printing of castables and (ii) the energy and thermal management of steel ladles.

Tools and their uses

These skills are often originated and commonly applied to distinct areas of knowledge. On one hand, this promotes multidisciplinary interactions, but usually at the price of demanding a self-taught strategy. Aiming to make this learning process easier, Fig. 1 describes one of the many likely roadmaps to achieve the mastery of these tools by the Refractory Engineer of the Present and the Future (REPF).

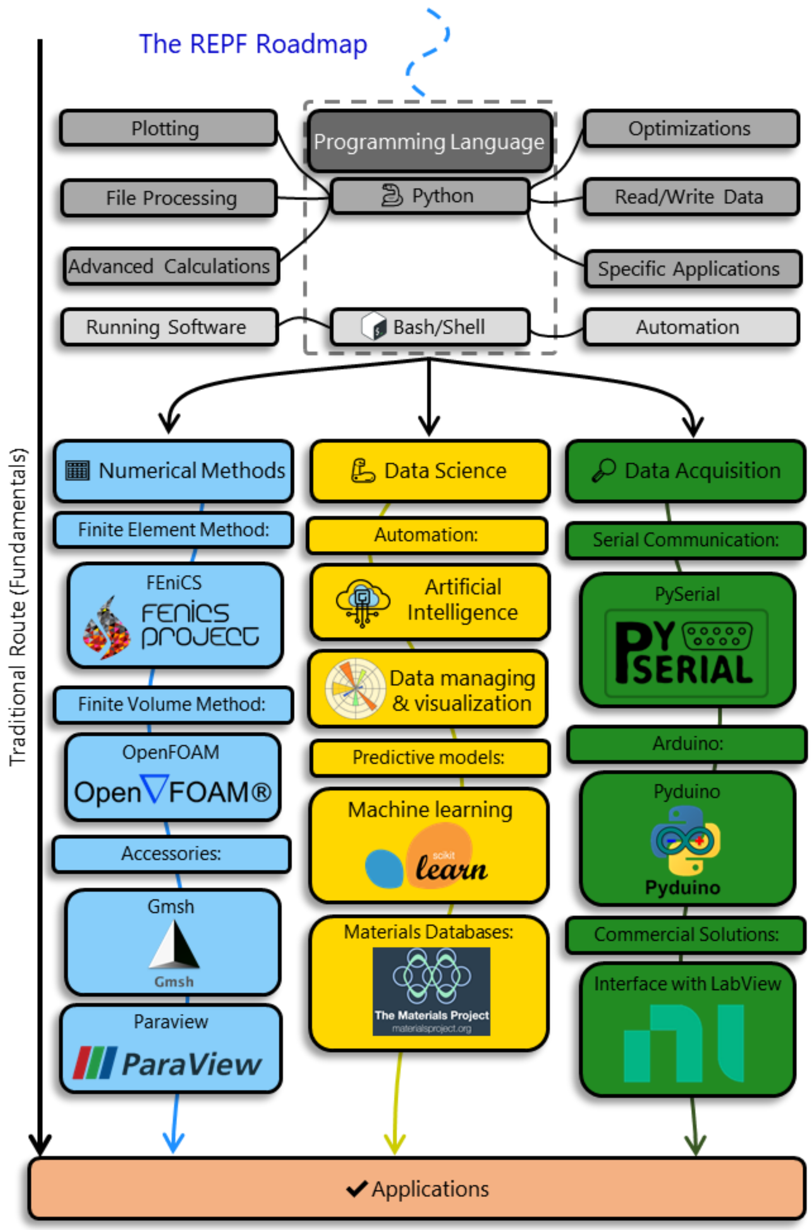

Fig. 1. The roadmap for the refractory engineer of the present and the future.

The current stage of maturity of software commonly used by the engineering mainstream is very noticeable by the intuitive graphical user interfaces available in many different applications, such as CAD tools and even the operating system itself.

However, for advanced tasks, learning a programming language might be extremely helpful and even mandatory in some cases. Thus, the REPF roadmap starts with two distinct ones. Python is an interpreted, high-level object-oriented programming language, used in several applications, but mostly known by the scientific community[5]. It recently became one of the most used languages, given its versatility. Python is free, as are its various learning resources, such as books, courses and videos. However, one should know that one of its main criticisms is that its computational costs on loops are high when compared to other compiled programming languages such as C++[6]. It should also be observed that solutions for it are common, such as using APIs (Application Protocol Interface) to integrate a Python interface with a fast C++ back-end, such as the case of the FEniCS Finite Element Method framework[7].

Secondly, Bash (also known as “Shell”) programming language is also highlighted as a valuable tool, as it is the most straightforward way to run software programs and to automate tasks on the command line interface.

The main applications for Python according to the roadmap are for preparing advanced plots (substituting expensive commercial software, such as Excel and Origin), for batch file processing and advanced calculations (such as polynomial fittings, statistical analysis, time-series investigations, signal processing, etc.).

Having consolidated this first set of skills, three branches can be pursued depending on the profile of the user, the problem at hand and the strategy of the solution. They are: (i) the numerical methods route, (ii) the data science track, and finally, the (iii) data acquisition path.

The numerical methods route comprises a strong mathematical background. This is the price of migrating from commercial applications to open source-based solutions. The learning curves are steeper and the understanding of the underlying theory is not optional. This directly affects the development timeline, but it can also lead to a more in-depth analysis and innovative findings. Another aspect is that niche problems commonly found in the refractory field are usually not present in commercial software. Thus, in some cases, open-source programs are the only option.

Two distinct numerical methods are presented in the roadmap: the Finite Element (FEM) and Finite Volume (FVM) methods, based respectively on the FEniCS platform and on the OpenFOAM software.

FEM is a numerical method for solving Partial Derivative Equations (PDE) based on searching for the best approximations of the analytical solution in a finite element function space, by multiplying the resulting PDE by a test function and integrating it over the domain of interest. This requires a mesh for spatial discretization. There are several open-source applications that can be used to create 2D and 3D meshes, but due to the ease of using it and the possibilities of parametrization, the selected tool for the REPF roadmap would be gmsh.

To solve the FEM problem, FEniCS[6] platform is the selected tool of choice due to important aspects such as documentation, the size of the community using it and versatility. For the post-processing stage, both Python itself (via libraries such as Matplotlib and meshio) and Paraview can be successfully applied for advanced visualization of the results.

Regarding the FVM method, the reasoning behind the technique relies on using the conservation equations for subpartitions of the domain of interest. By enforcing the continuity laws for the mass, thermal energy and momentum fields, one can obtain a linear system of equations. For this technique, OpenFOAM[8] is the most versatile and comprehensive open-source software, with applications ranging from Computational Fluid Dynamics, (CFD), combustion analysis, even financial problems. Once more, gmsh, Python and Paraview can be used for mesh creation and visualization of results.

Using this package, complex problems on heat transfer while operating refractory lined equipment can be carried out starting from the geometry definition, followed by mesh preparation, solution of the system of equations, and finally finishing with post-processing. The analysis can also be focused on different aspects of the refractory field, ranging from the computation of effective properties to the simulation of a whole industrial process, such as steel cleaning by ceramic filters[9].

The data science track has its roots in the most crucial asset of the century: data. Recently established Internet companies have shown that they can capitalize unimaginable volumes of investments by efficiently managing the data they collect from their community. The amount of data they analyze would be impossible for human teams, therefore this capability was exponentially increased by artificial intelligence software.

Not only the Silicon Valley companies noticed this trend. Traditional and well-established industries have been drastically shifting their business strategies to adapt all data technologies to their operations. Many strategies will connect them to all increasing data production already coming from their facilities, by using sensors and a more sophisticated analysis for processing optimization and controlling, which are the other branches in the REPF roadmap.

The robust data analysis pipelines can provide enough information for process automation and assertive decision-making. The machines are constantly evaluating all the relevant data that will lead to actions to reduce costs and maintenance, increase productivity, etc. These are the goals when solving refractory development, production or application problems.

Since the first PCs and operational systems, commercial data analytics software has been available. For instance, Microsoft Excel and its spreadsheets are the best tool of most industries' data analysis. Indeed, they can provide rich information when handling low dimensionality data. However, if the expectations were to find statistical correlations on high dimensional spaces and datasets, such spreadsheet software would become very limited.

The complexity of industrial processes, especially the ones at high temperatures, depends on many different factors. In these cases, there is not much available commercial software that will manage directly with data, especially if the latter are recorded inappropriately. The engineer in these cases might look for programming languages, as in the case of Python, which provides a package of libraries to support the REPF to analyze complex data problems.

A great set of packages would include Pandas, Numpy and Scipy for data preparation and structuring. The first one is an open-source library providing high-performance, easy-to-use data structures and data analysis tools[9]. Numpy and Scipy are a set of fundamental packages for scientific computing. Numpy provides algorithms for optimization, integration, interpolation, eigenvalue problems, algebraic equations, statistics and many others[11].

For data visualization and dashboard design, Matplotlib or Seaborn are the most common libraries for creating static, animated and interactive visualization[12]. The understanding and usefulness of data are more remarkable when industrial information undergoes such analysis, especially when considering the development of smart systems, as it requires high-quality data to build predictive models as obtained by machine learning tools.

The Python library that provides the most practical algorithms for machine learning is Scikit Learning. It can be applied for supervised and unsupervised learning, in the context of classification or regression problems. For instance, a regression problem for refractory application would be the lining thickness prediction in the basic oxygen furnace (BOF) according to the specific conditions of the process[13]. In the same environment, a classification example could be to identify cracks in refractory linings by image analysis.

First-principles generated databases of materials' properties are also an essential source of information, which can be queried by using Python APIs. One of the most extensive representations of this is Materials Project[14].

Finally, the data acquisition path can also be pursued. This set embodies tools that can be used with legacy versions of equipment through serial communication (using the PySerial library), custom state-of-the-art electronic platform (via Pyduino) and even interaction with commercial solutions such as LabView. This can be used to develop custom-made laboratory equipment and even be scaled up to industrial applications.

This leads to information streams that can successfully feed the data science algorithms, as well as to characterize the behavior of the materials during applications, providing important information for the validation of numerical models.

All these three paths in Fig. 1 are closely interconnected and can provide innovative insights. One critical comment is that the full mastery of each of these individual tools takes years of experience, and what is proposed by this roadmap is to provide the basic knowledge to start and create connections with the real experts in each of these areas. Nevertheless, we should never underestimate nor neglect the fundamentals of refractory engineering and the working experiences, which are unique to professionals in this area of knowledge.

Finally, the low initial investment of these tools promotes easier prototyping of solutions, which directly increases the likelihood of innovations. Furthermore, the fact that these open-source tools rely on a strong fundamental background makes the experience of working with them a rich environment for active learning.

Thus, the next section presents a couple of examples of tool applications presented in the REPF roadmap. It is a conceptual exercise that shows how a challenging innovation can be approached from these tools. This, however, does not overlook the helpful contributions of proprietary commercial software, nor the pivotal importance of the fundamentals necessary to understand these challenges.

Example of applications

3D Printing of refractories

Refractory insulating materials are one of the key elements for improving the energy efficiency of high-temperature processes by enhancing energy conservation through low thermal conductivity. This property is usually obtained using porosity as a way to decrease thermal energy transport. It is well known that the porosity itself is not enough to control the thermal conductivity of a material, especially at high temperatures, when radiation increases energy losses[15]. One strategy is to rely on hierarchical structures[16]. Thus, methods to control and manufacture optimized porous refractory materials are critical. Several options are actively being researched and one of the most promising ones is Additive Manufacturing (AM). In this example, using 3D printing as a methodology to optimize the pore size and its distribution at hierarchical scales is discussed.

Fig. 2 describes an overview of the main challenges of this development, as well as the main tools that could be applied for each stage.

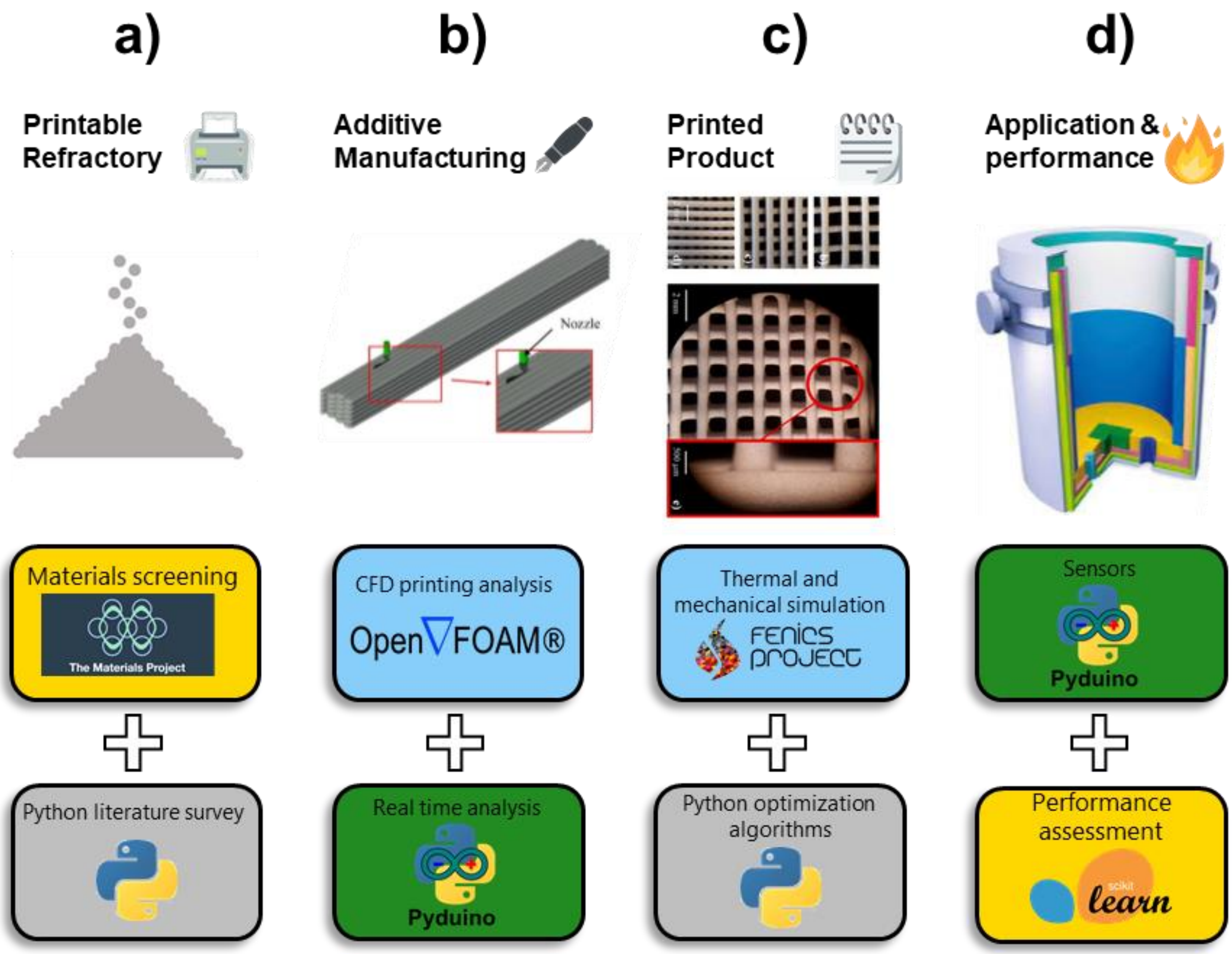

Fig. 2. An example of the application of REPF skills for the additive manufacturing of hierarchy porous insulating refractories. Adapted from Steiner et al.[17] and Coppola et al.[18].

Starting with the printable refractory composition in Fig. 2-(a), the selection of raw materials and additives is a complex task. Several routes are available to optimize the rheological behavior of ceramic suspensions[19]. Fundamentals are helpful to understand the likely routes to stabilize these slurries. However, the ever-growing list of likely candidates of dispersants makes selecting the best one a complex challenge. Thus, it is proposed using a high throughput strategy where both materials databases (such as the Materials Project) and literature surveys on indexed databases are applied. These tools have APIs where Python scripts can be used to automate tasks and search for thousands of materials, yielding a list of likely candidates. The rheological properties of the resulting slurries can then be characterized and match the suitable viscosity, yield strength and its non-Newtonian behavior necessary for successful printing.

Having selected the correct composition, the next stage is the additive manufacturing itself, depicted in Fig. 2-b). For the sake of simplicity, the current example will only focus on the Direct Ink Writing (DIW) technique. For the DIW, the main parameters of control are the flow rate through the nozzle, its velocity, the infill percentage and the orientation of the printed strands. Once more, this leads to an optimization problem. One strategy is to experimentally test a set of combinations of these parameters and select the procedure with the best resulting material. To do this, real time analysis can be of great interest. Given the digital nature of additive manufacturing, a Python script could be used to set multiple tests and an automatic set of sensors could be controlled through an Arduino to gather information on the parameters of interest. This, however, can be costly, take too much time and also miss better combinations that were not present in this initial set of combinations. Thus, it can be proposed either as a combination or as a substituting strategy, using CFD analysis (using OpenFOAM) to simulate the rheological behavior of the suspension during the AM process, as described in Fig. 2-(c).

The resulting material at the end of the processing route can be characterized, giving special attention to its thermal and mechanical properties. As 3D printing depends on several parameters (percentage of infill, printing directions, layer thickness and others) that directly affect the final properties, numerical simulations could be used to guide the selection of the target structure with the lowest effective thermal conductivity and highest strength. To do this, FEniCS can be used to solve the FEM problems for heat transport and the mechanical behavior of the resulting material. Using optimization algorithms could further improve the performance of the structure and provide the desired property.

Finally in Fig. 2-(d), the application could be assessed by both numerical tools (not represented in Fig. 2), and specially by using a combination of sensors and machine learning algorithms. This could provide further insights into the desired materials and feed them back to the selection of the refractory composition and the processing conditions.

This example of the AM processing route for insulation refractory materials is only an overview. Certainly, other aspects which were not addressed here would necessarily be considered (economic implications, likely reduction on the CO_2 emissions, productivity of the processing route, etc), but it nevertheless illustrates how the tools presented in the REPF roadmap can complement the fundamentals and offer novel perspectives that speed-up the innovation in the refractory field.

Energy and thermal management of steel ladles

The thermal and energy management of the steel ladle process is another example of applying open-source computational tools for solving refractory-related problems. This is an essential issue in the steelmaking process, driven by the refractory lining features and operation management. The secondary metallurgy stage in steelmaking adjusts the final composition and the temperature of the liquid steel before pouring it into the mold (or starting the continuous casting process), and all these corrections take place in the steel ladle. Due to the strict requirements and high productivity, the steel ladle operation is complex and fundamental for achieving the metallurgical goals. Most of these requirements depend on the thermal condition and energy balance between the refractory lining, the liquid steel, the heating sources (for the lining and molten steel) and the environment.

The relevance of the refractory lining is straightforward. It holds the liquid steel during the secondary metallurgy to convey and refine the steel in the industrial site. Besides ensuring the integrity of such an operation, one of the primary roles of the refractory lining is to keep the molten liquid steel at the desired temperatures, avoiding unnecessary reheating and guaranteeing the efficiency of the refining steps. The liquid steel temperature dictates several actions in the steelmaking shops because of its close relation to the final product quality and productivity.

For instance, to avoid severe temperatures changes in pouring the liquid steel in the ladle, the lining needs to be heated up, minimizing the temperature gradient between the room temperature lining and the high-temperature liquid metal. If the temperature of the liquid steel drops to certain low levels depending on the steel shop protocols, there will be an additional step in a reheating station to avoid undesired solidification. Any of these heating steps, when required, would consume energy and spend time, which indeed might be avoided or optimized[3].

In this context, the application of open-source computational tools helps the REPF to manage the steel ladle's thermal and energy balance. Figure 3 introduces four of these tasks related to the refractory and the heat management of the steel ladle, connecting them to the tools listed in Figure 1. Several other discussions and strategies could be drawn, such as the application of such devices from the metallurgical point of view, nevertheless, herein the analysis will focus on the refractory perspective.

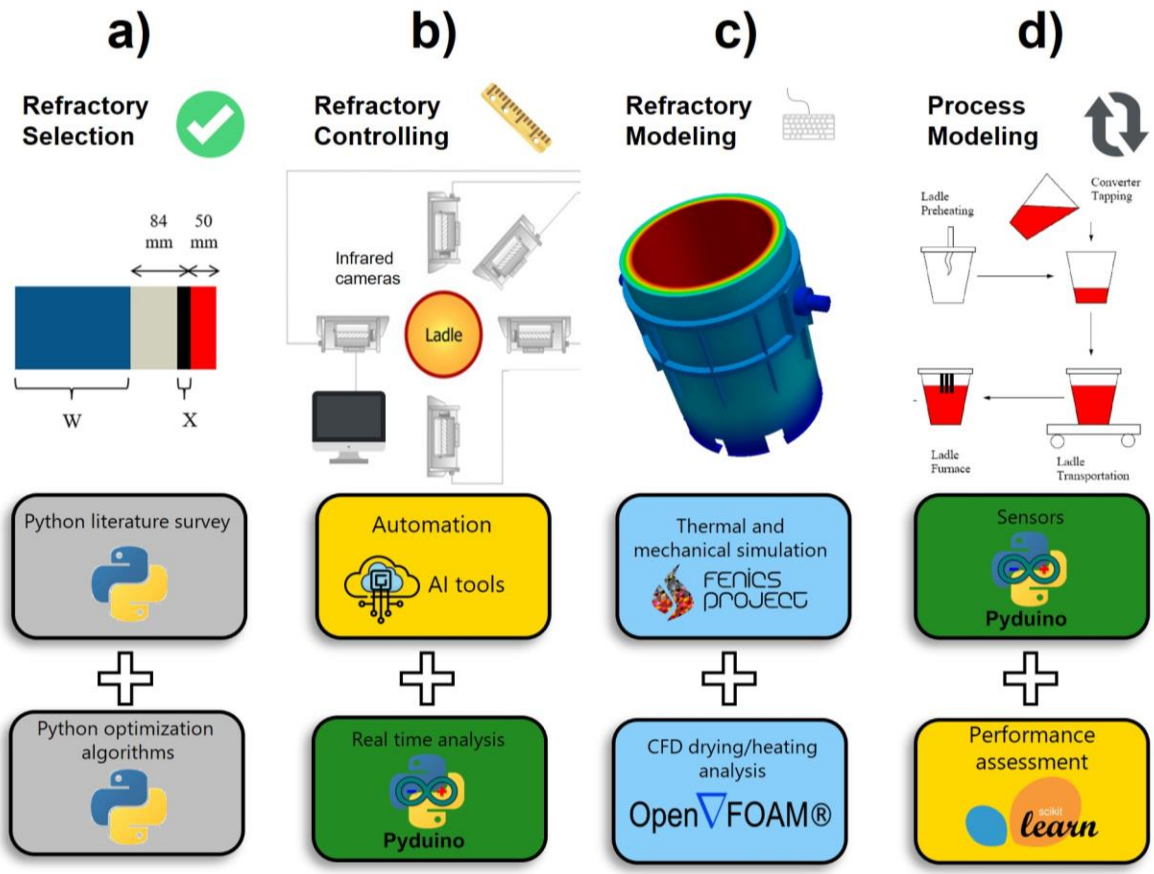

Fig. 3. An example of the application of REPF skills for the energy and thermal management of steel ladles, which includes the performance of refractories

Figure 3-a) presents one fundamental task for the thermal and energy management of the steel ladle, which consists of selecting the suitable refractory materials for lining the vessel’s metallic shell. According to expected performance, many products and refractories can be applied to the lining. In the case of the steel ladle, the lining is usually multi-layered and zoned. A simple example can be a refractory selection for the steel ladle wall. Usually, the refractory lining in this region consists of three to five layers with different materials. Each layer will demand specific refractories to meet the different corrosion requirements, operation temperature and life span needed. Furthermore, each layer’s thickness can impact the steel ladle's thermal efficiency and its available capacity. The strategy for selecting the best lining configuration, taking as many factors as possible, acknowledges the application of optimization algorithms coupled to refractory property databases (literature surveys or datasheet gathering).

Santos et al.[20] proposed making the refractory selection of a lab furnace considering different lining thicknesses, thermal properties and materials costs. The optimization involved genetic algorithms (chosen to decrease the search space and reduce the search time) associated with heat transfer models. The best configuration from the search space was selected considering the lower energy consumption and cost, while maintaining the working capacity of the furnace. Experimentation and testing for these optimization problems would be costly and sometimes even impossible for engineers with traditional backgrounds.

In the case of Figure 3-b), another task can be solved after combining open-source computational tools. The example illustrates a strategy for monitoring and controlling the refractory performance, especially for unexpected failure, by constantly recording the steel ladle shell temperatures via infrared sensors. This online temperature measurement allows the operation to forecast hot spots and repair the lining at a suitable time[21]. The hot spot results from intense heat transfer throughout the refractory lining, indicating an abrupt thickness reduction or a crack infiltration. The predictions in this case only make sense if the temperature is constantly monitored and the data analysis is carried out almost instantaneously. If any steel leakage happens, the consequences can be catastrophic for the finances and security. Infrared sensors are essential for high-temperature processes because they can work in harsh environments and make contactless temperature measurements possible.

Another critical task in dealing with the thermal and energy management in the steel ladle process is modeling (Figure 3-c). Simulation of physical phenomena as the heat transfer in high temperatures processes is challenging, but its outputs foster many optimization and innovative solutions.

Predicting and modeling the temperature distribution in the steel ladle process can be as simple as obtaining the temperature profile in the walls while the system is in stationary thermal condition or as complex as modeling the radiative heat transfer during heating the lining and its impacts on the drying behavior of the refractory installed. For instance, the latter has been investigated in depth. Some authors, such as Murilo et al.[22], showed a mixed formulation accounting for the heat and mass transfer inside the material, which can help the REPF to predict the faster and lower energy consumption heating schedule. Their model was developed with an open-source FEM tool, FEniCS, and it allowed the investigation of different materials under distinct operational conditions. The optimization of heating schedules can improve the steel ladle availability reducing the time spent. As mentioned, it can reduce the energy consumption for heating the refractory.

The latter presented task consists of applying open-source tools to determine the steel ladle's steel temperature during the secondary refinement (Figure 3-d). Several strategies could be suggested for modeling the process. Herein, the use of sensors and machine learning are highlighted. The strategy is based on the study by Viana Jr.[23], who coupled thermodynamic models with artificial neural networks to predict the steel temperature from tapping the basic oxygen furnace to the continuous casting machine. The resulting model considered several operational parameters as the time of each refinement step (tapping, stirring, gas removal, reheating), the intensity of every process (e.g., gas flow while bubbling), the thermal losses to the refractory lining, and many others. Each of the predictions were carried out online and depended on the temperature measurements collected throughout the operation.

The effort in predicting the steel temperature comes from the lack of sensors that could potentially continuously measure the temperature and not only once in while during the process.

Conclusions

Finding solutions for complex problems requires upfront technologies and fundamentals from different fields. The engineering background in the refractory and materials science areas is shifting to a complex system engineering background, which can understand the abstract connection among the areas of knowledge and develop solutions upon them.

Globalization and the Internet have significantly helped this change, as they universalized many of the tools and knowledge to understand them, freely, as open-source tools and learning spaces. The REPF is on course!

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