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

M. F. Santos[a,*], M. H. Moreira[a], V. C. Pandolfelli[a].

[a] Federal University of Sao Carlos, Graduate Program in Materials Science and Engineering, São Carlos, São Paulo, Brazil.

* matheusfesan@gmail.com

ABSTRACT

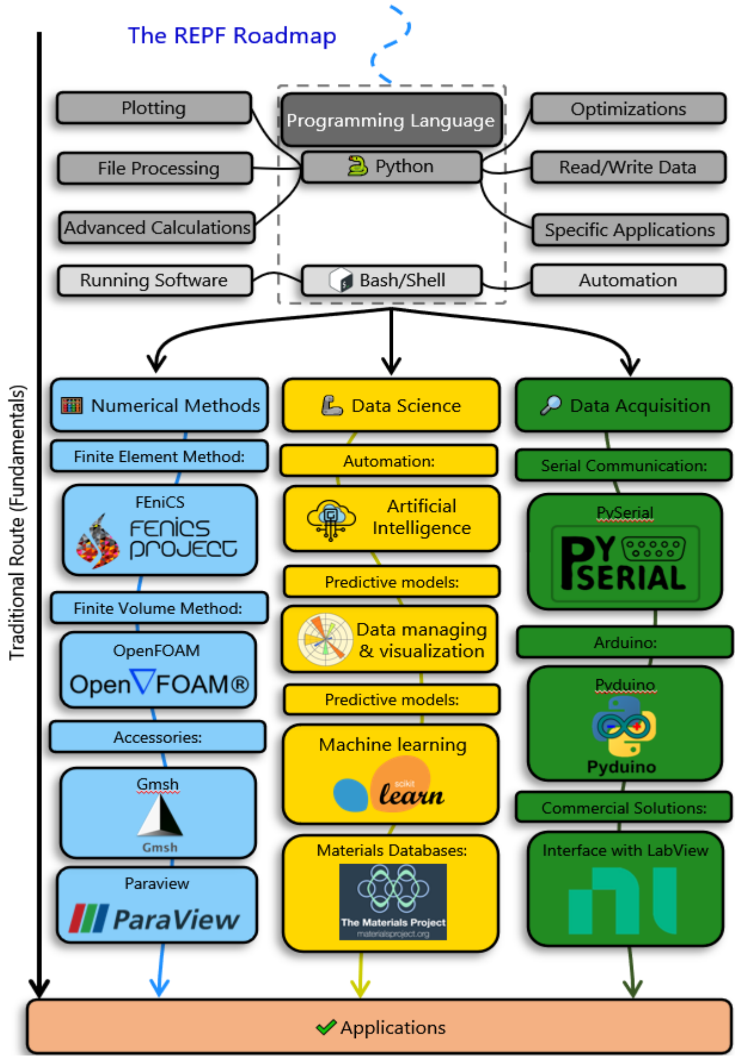
The world has physically and virtually changed by innovations as shown for the transportation (engines, airplanes) to communication (with phones, internet, and satellites among many others). These technology advances were able to reshape society and the set of skills required for the young professionals have been dramatically shifting. The refractory industry is demanding those who understand this new world and can solve its challenging problems. The complexity of materials knowledge includes the latest advances in modeling and data science, which requires a sophisticated blend of fundamental concepts and advanced techniques. 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 the present and future professionals. As a conclusion, the package of skills is presented considering the association of industry, academics, students, and computing, to synergistically and fundamentally solve the new world's challenges, promoting true, open and consistent innovation.

1 INTRODUCTION

Refractories are a category of materials able to withstand challenging conditions, ranging from high temperatures, high chemical activity and great mechanical loads[1]. The current scenario of worldwide efforts to minimize the environmental impacts of human activities[2] is adding a new dimension for the optimization of the refractories: besides sustaining their function in harsh environments, it must also do so with minimal carbon footprint while also yielding the highest possible energy efficiency by diminishing thermal losses, for instance[3].

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

In this context, the current work aims to propose how the current challenges on the



innovations on refractory can be developed by linking fundamentals and digital tools, which could be critical for the new generations of refractory engineers. These skills are often originated and commonly applied to distinct areas of knowledge. On one hand, this promotes multidisciplinary interactions, but at the price of often demanding a self-taught strategy. With the purpose 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).

The current stage of maturity of the software commonly used by the engineering mainstream is very noticeable by the very intuitive graphical user interfaces available for most different applications. However, for advanced tasks, programming language knowledge might be extremely helpful and even mandatory in some cases. Thus, the REPF roadmap starts with two distinct programming languages. Python is an interpreted, high-level object-oriented programming language, used in several applications, but mostly known by the scientific community[4].

Python is free, as well as 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 during loops are high when compared to other compiled programming languages such as C++[5]. It should also be noted that solutions for it are common, such as using APIs to integrate Python's interface with a fast C++ back-end, such as the case of the FEniCS Finite Element Method framework[6]. 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.

The main applications for Python according to the roadmap are its use for preparing advanced plots, for batch file processing and advanced calculations (such as polynomial fits, statistical analysis, etc.). Special attention to optimization algorithms as well as specific applications is also described. With this first set of skills consolidated, three branches can be pursued depending on the user profile, 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. The learning curves are steeper and the understanding of the underlying theory is not optional. This directly affects the timeline of development, but it also can lead to deeper analysis and more 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 the Finite Volume (FVM) methods, based respectively on the FEniCS platform and on the OpenFOAM software. FEM is a numerical method of solution of Partial Derivative Equations (PDE) based on the search of the best approximations of the analytical solution in a finite element function space, by multiplying the resulting PDE with a test function and integrating it over the domain of interest. This requires a mesh for spatial discretization. For the solution of the FEM problem, the FEniCS[6] platform is the selected tool of choice due to important aspects such as documentation, size of the community using it and versatility. For the post-processing stage, both Python itself (through libraries such as Matplotlib and meshio) and Paraview, can be successfully employed 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[7] is the most versatile and comprehensive open-source software, with applications ranging from Computational Fluid Dynamics, (CFD), combustion analysis, to even financial problems. With this package, complex problems on heat transfer during the operation of refractory lined equipment can be carried out. 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 the filtration of steel by ceramic filters[8].

The data science track has its roots in the most important asset of the century: data. Not only the Silicon's 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. There are many strategies that will connect to all the increasing data production already coming from the installations, due to the set of new sensors, to more sophisticated analysis for processing optimization and controlling, that are basically the other branches in the REPF roadmap.

The robust data analysis pipelines can provide enough information for process automation and assertive decision-making, as the machines are instantly and constantly evaluating all the relevant data that will drive actions to reduce costs, reduce maintenance, increase productivity, etc. These are goals when solving refractory development, production or application problems. Commercial data analytics software has been available since the first PCs were developed. For instance, Microsoft Excel and its spreadsheets are the best pictures of data analysis of most industries nowadays.

The complexity of industrial processes, especially the ones at high temperatures, is dependent on a lot of different factors. In these cases, there are not many available commercial software that will be able to deal directly with data, especially if they are stored 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 analyzing complex data problems. One great set of packages would include Pandas, Numpy and Scipy for data preparation and structuring. The first is an open-source library providing high-performance, easy-to-use data structures and data analysis tools[9]. The second and third are part of the fundamental packages for scientific computing. The last one provides algorithms for optimization, integration, interpolation, eigenvalue problems, algebraic equations, statistics and many others[10].

For data visualization and dashboard design as Matplotlib or Seaborn[11]. Scikit Learning is the Python library that provides most of the useful algorithms for machine learning. 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[12]. In the same environment, a classification example could be the identification of cracks on refractory linings by image analysis. First-principles generated databases of materials' properties are also an important source of information, which can be queried by using Python API's. One of the largest representations of this is the Materials Project[13].

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 (by the aid of 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 laboratory equipment and even be scaled-up to industrial uses. 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 the numerical models.

All these three paths are tightly 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 have the basic knowledge to start and create connections with the real experts in each of these areas. This collective problem-solving strategy relies on effective connections between the experts but never underestimating nor neglecting the fundamentals of refractory engineering, which are unique to the professionals of this area of knowledge. Besides, without a preliminary notion of the capability of these open-source solutions, one might be unable to detect opportunities for process improvements or new ideas.

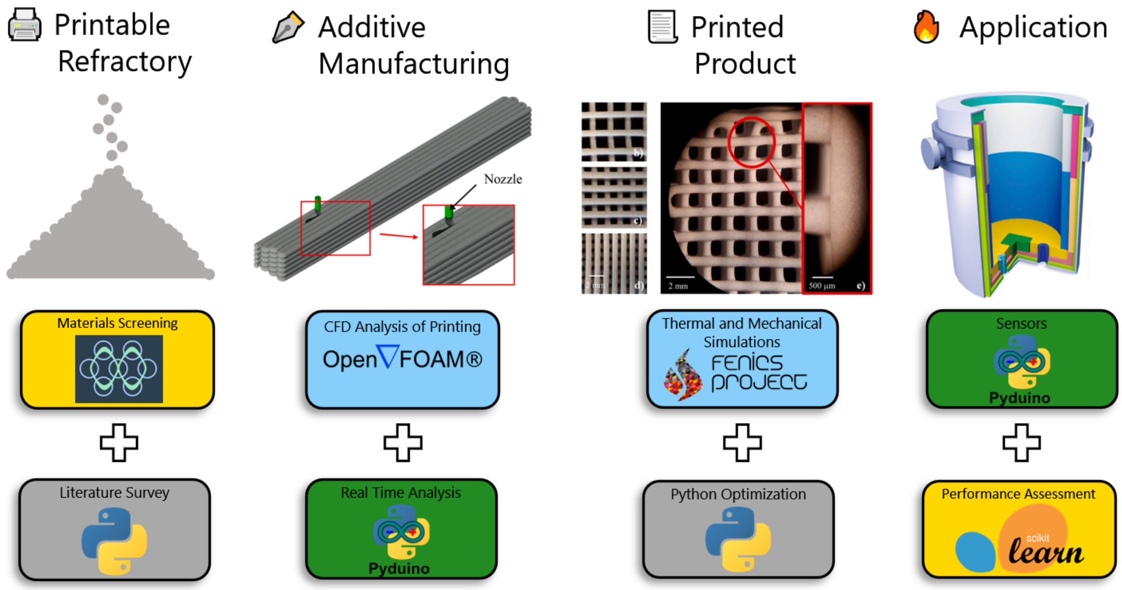
Finally, the low initial investment of these tools promotes easier prototyping of solutions, which directly increases the probability of encountering novel solutions. Also, the fact that these open-source tools rely on a strong fundamental background makes the experience of working with them a rich environment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

Thus, the next section presents an example of the application of the tools 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 ignore the helpful contributions of proprietary commercial tools, nor the pivotal importance of the fundamentals necessary to understand this challenge.

2 EXAMPLE OF APPLICATION

Refractory insulating materials are one key element for the efforts on improving the energy efficiency of the high-temperature processes by enhancing energy conservation through low thermal conductivity. Such a 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 starts to be a major share of the energy transport process[14]. One strategy is to rely on hierarchical structures[15].

Fig. 2. Example of application of skillets of the REPF for the additive manufacturing of hierarchy porous insulating refractories. Adapted from [16] and [17].



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 by using of Additive Manufacturing (AM). In this example, 3D printing is shown as a methodology to optimize the pores sizes and distribution at hierarchical scales. 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. Starting from the printable refractory composition, the selection of raw materials and additives is a complex task. Several routes are available to optimize the rheological behavior of ceramic suspensions[18]. Fundamentals are helpful to understand the likely routes to stabilize these slurries.

However, the ever-growing list of likely candidates for using as dispersants renders the selection of 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. Such tools have APIs where Python scripts can be used to automate tasks and search for thousands of materials. With the correct composition selection, the next stage is the additive manufacturing itself. For the sake of simplicity, the current example will be only focusing on the Direct Ink Writing (DIW) technique.

For this route, 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. For that, real time analysis can be of great interest. Given the digital nature of additive manufacturing, a Python script could be used to carry out 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, takes too much time and miss better combinations that were not present in this initial set of combinations. Thus, it can be proposed either as a blend or as a substituting strategy, the use of CFD analysis (using OpenFOAM), to simulate the rheological behavior of the suspension during the AM process.

The resulting material at the end of the processing route can be characterized, with special attention to its thermal and mechanical properties. As 3D printing offers several parameters that directly affect such properties, numerical simulations could be used to guide the selection of the target structure with the lowest effective thermal conductivity and highest strength. For this, FEniCS can be used to solve the FEM problems for heat transport and the mechanical behavior of the resulting material. The use of optimization algorithms could further automatically improve the performance of the structure and provide the desired optimized property. Finally, the application could be assessed by both numerical tools (not represented in Fig. 2 for brevity), and specially by using a combination of sensors and machine learning algorithms. This could provide further insights on 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 approached 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 new perspectives that facilitate the innovation in the refractory field.

3 CONCLUSIONS

Relevance for 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 between the areas of knowledge and develop solutions upon them. Globalization and the internet have helped significantly to this change, because they universalized many of the tools and knowledge to understand them, freely, as open-source tools and learning spaces. The REPF is on course!

4 ACKNOWLEDGEMENTS

This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES) - Finance Code 001 and Fundação de Amparo à Pesquisa do Estado de São Paulo - FAPESP (grant number: 2021/00251-0). The authors are also greatly thankful for FIRE support in this work.

5 REFERENCES

1. C. Schacht, Refrac. Handbook, Mechanical Engineering, CRC Press (2004)
2. V. Masson-Delmotte, IPCC: Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change, P. Zhai et al. Cambridge University Press. In Press. (2021)
3. M. F. Santos, et al., Enhanced numerical tool to evaluate steel ladle thermal losses, Ceramics International [44] pp. 12831-12840, (2018)
4. E. T. Oliphant, Python for scientific computing. Computing in Science & Engineering [9.3] pp. 10-20 (2007)
5. R. Pereira, et al, Energy efficiency across programming languages: how do energy, time, and memory relate. In Proceedings of 2017 ACM-SIGPLAN International Conference on Software Language Engineering. ACM, New York, NY, USA, (2017)
6. M. S. Alnaes, et al., The FEniCS Project Version 1.5, Archive of Numerical Software [3] (2015)
7. H. Jasak, OpenFOAM: open source CFD in research and industry. International Journal of Naval Architecture and Ocean Engineering. [1]. pp. 89-94, (2009)
8. A. Asad, et al., Numerical investigation of the combined effect of reactive cleaning and active filtration on inclusion removal in an induction crucible furnace. Steel Research International. [92]. (2021)
9. W. McKinney, Data structures for statistical computing in Python, Proceedings of the 9th Python in Science Conference, Volume 445, pp. 56-61, (2010)
10. P. Virtanen, et al., SciPy 1.0: Fundamental algorithms for scientific computing in Python. Nature Methods, 17(3), pp. 261-272 (2020)
11. J. D. Hunter, Matplotlib: A 2D Graphics Environment, Computing in Science & Engineering, vol. 9, no. 3, pp. 90-95,(2007)
12. M. Forrer, Prediction of refractory wear with Machine Learning Methods, Master Thesis, Graz University of Tecnology, (2012).
13. A. Jain, et al., The Materials Project: A materials genome approach to accelerating materials innovation, APL Materials, 1 [1], pp. 011002, (2013)
14. P. I. Pelissari, et al., Analysis and modeling of the pore size effect on the thermal conductivity of alumina foams for high temperature applications. Ceramics International. [43] pp. 13356-13363, (2017)
15. N. Kleger, et al. Hierarchical porous materials made by stereolithographic printing of photo-curable emulsions. Sci Rep 11, pp. 22316 (2021)
16. R. Steiner, et al., Refractories 4.0, BHM Berg-und Hüttenmännische Monatshefte, 162, [11], pp. 514-520, (2017)
17. Coppola, B., et al., 3D printing of dense and porous alkali-activated refractory wastes via Direct Ink Writing (DIW). Journal of the European Ceramic Society, 41, [6], pp. 3798–3808, (2021)
18. A.P. da Luz, M.A.L. Braulio, V.C. Pandolfelli, Refractory Castable Engineering, vol. 756, Goller Verlag GmbH, Baden-Baden (2015)